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Pandora Technical Description and User Guide

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Working Reports contain information on work in progress or pending completion.

The conclusions and viewpoints presented in the report are those of author(s) and do not necessarily coincide with those of Posiva.

ABSTRACT

Pandora is an extension of the well-known technical computing and simulation software MATLAB and Simulink of The Mathworks Inc.

Pandora was developed to simplify development of models resulting in large systems of differential equations where decay of radionuclides is included in the model and to enhance the graphical user interface to be more suitable for radioecological modelling.

MATLAB is a programming language and a computing environment. It provides core mathematics and advanced graphical tools for data analysis, visualisation, application development etc. Simulink is mainly targeted at modelling and simulating dynamic systems. Simulink provides a block diagram interface for MATLAB. Pandora facilitates effective use of them for radionuclide transport modelling.

In the report the technical solutions of Pandora are outlined through a presentation of the key elements and a step-by-step sample case serving also as a user guide.

Keywords: *biosphere modelling, simulation tool, dose assessment.*

PANDORA - TEKNINEN KUVAUS JA KÄYTTÖOHJE

Pandora on laajennus tunnettuun The Mathworks Inc:n teknisen laskennan ja simuloinnin ohjelmistoperheeseen, jonka muodostavat MATLAB ja Simulink.

Pandora kehitettiin yksinkertaistamaan laajoja differentiaaliyhtälöitä ja radioaktiivisia hajoamisia ja hajoamisketjuja käsittävien mallien kehittämistä sekä parantamaan graafista käyttöliittymää paremmin radioekologista mallinnusta palvelevaksi.

Tässä sovelluksessa MATLAB toimii ohjelmointikielenä ja laskentaympäristönä, joka tarjoaa laskentarutiinit ja edistykselliset graafiset työkalut data-analyysiä ja visualisointia varten. Simulink on tarkoitettu pääasiassa dynaamisten järjestelmien mallintamiseen ja simulointiin, ja se muodostaa lohkokaaviotyyppisen käyttöliittymän MATLABiin. Pandora puolestaan helpottaa radionuklidien kulkeutumismallinnusta näitä perustyökaluja soveltaen.

Tässä raportissa kuvataan Pandoran tekninen toteutus esittelemällä sen avainosat sekä käymällä vaihe kerrallaan läpi esimerkkimallin rakentaminen tässä ympäristössä, mikä toimii samalla Pandoran käyttöohjeena.

Avainsanat: *biosfäärimallinnus, simulointi, annosarviointi.*

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1 INTRODUCTION

The Finnish and Swedish radioactive waste management companies, Posiva and SKB, are currently endeavoured in a programme for the safe disposal of high-level radioactive waste generated by nuclear power plants. An important task in this programme is the assessment of the safety for man and the environment of the proposed technological solution (e.g. SKB 2004, Vieno & Ikonen 2005). As part of the safety assessment, it is necessary to make prognoses of the biosphere evolution and the environmental behaviour of radionuclides under very long-term periods, lasting thousands of years. Such prognoses will have to rely on multiple-interfaced models that can handle diverse biosphere conditions and scenarios involving climatic and other environmental changes.

The model development will have to involve experts in multiple disciplines and its continuous development is envisaged, which will incorporate new knowledge and data obtained from on-going site investigations and research programmes. Consequently, it would be convenient to develop the models using a common modelling tool that allows implementing a modular structure, which can be shared by various users and be continuously upgraded.

Several existing commercial codes were considered, and after analysing advantages and disadvantages, the Matlab/Simulink© software was chosen as the platform for developing the modelling tool. Simulink© is a highly flexible tool that can be used for simulations of practically any type of dynamic system, with a graphical model description. Models developed in Simulink© can easily be combined with procedures or models written in common programming languages, such as Fortran and C++. Matlab/Simulink© is a commercially transparent environment, widely used within the scientific and engineering community and is continuously upgraded. A drawback, though, is that substantial experience and effort is required to implement a model, and to take advantage of all available capabilities. Moreover, users not familiar with Simulink© may have difficulties to understand and run models implemented by others.

In order to make the Matlab/Simulink© platform more easy to use, whilst keeping its advantages, a library of Simulink© blocks and a toolbox for facilitating the creation and handling of radioecological models, called Pandora, were developed and implemented as an add-on to Simulink©. The Pandora tool comprises of a library of Simulink blocks and a free standing Manager.

This report is mainly a technical user guide of Pandora, but it also presents the tool in general. An step-by-step implementation of a test model is also described for an example. It is assumed that the reader knows the basics of Matlab© and Simulink© environments. General overview on them is available e.g. at http://www.mathworks.com/.

Pandora is a unification of the projects BIOMAT developed by Facilia AB on contract to Posiva Oy within a co-operation project with Svensk Kärnbränslehantering AB (SKB) and TENSIT (Jones et al. 2004) developed by SKB.

2 PANDORA VERSION 1

The Pandora tool comprises of a library of Simulink blocks and a free standing interface, The "Pandora Manager", a utility to facilitate the implementation of radionuclide transport models in Simulink.

The following parts, described in more detail in chapters 3 and 4, are included in the Pandora (version 1.0) library:

- Radionuclide Manager (Pandora-block) – for handling decay and in-growth of several radionuclides.
- Constant+ block – for easier handling of possibly nuclide-dependent parameters.
- Parameter manager – used in conjunction with Constant+ block for central editing of values and distributions.
- Reservoir – for creation of compartments that can easily handle multiple radionuclide decay and in-growth data.
- Rate block to be used with Reservoir blocks to control flux between Reservoirs.
- Filter block – to filter out certain nuclides, signal dimensions are preserved.
- Selector block – to select certain nuclides, signal dimensions are reduced.
- Result Report Manager – for exporting named data to text files and/or Excel.
- Plot Manager – for representing named data in Matlab plot windows.
- Parameter Report Manager – for exporting system settings and model parameters to text files.
- Unit conversion blocks "bq2mole" and "mole2bq" for conversion of units between mole and becquerel.
- Inflow block – to represent inflow of contaminants to the model.
- Statistics blocks – to define result nodes in the model, when running probabilistic simulation.

All codes in Pandora are written in the Matlab and Java languages. Java is used only internally in Pandora and no knowledge of Java is needed to use Pandora. Some knowledge of Matlab is probably an advantage and basic knowledge of how to build block-based models in Simulink is required to use Pandora. Although one could build simple models (as the test case) with less experience, familiarity with Simulink is strongly recommended for making the simulation settings and connecting other non-basic blocks than the Pandora blocks to the model.

3 PANDORA TOOLS

The Pandora tool consists of two separate parts: the Pandora Manager and the Pandora library of Simulink blocks. The blocks in the library can be used independent of the Pandora Manager but the Manager facilitates the construction and maintenance of large models.

In this chapter, the Pandora Manager and controlling of model creation and simulation runs are presented. Chapter 4 introduces then the actual building blocks of the Pandora models, i.e. the block library.

3.1 Parameter handling through Excel sheets

The input of parameters in Pandora is done via Excel sheets. There are three different types of parameters handled by Pandora:

- Site-specific: Scalar local parameters e.g. lake area.
- Element-specific: Nuclide-dependent, or in general species-dependent, global parameters e.g. Kd.
- Universal: Scalar global parameters typically physical constants e.g. gravity.

Parameters are stored in Excel sheets, which in turn are pointed to in a main Excel set-up sheet for the model. An example of such a main sheet is shown in figure 3.1. The contents of this sheet can either be edited directly in Excel or through the parameters tab in the Pandora Manager (see section 3.3).

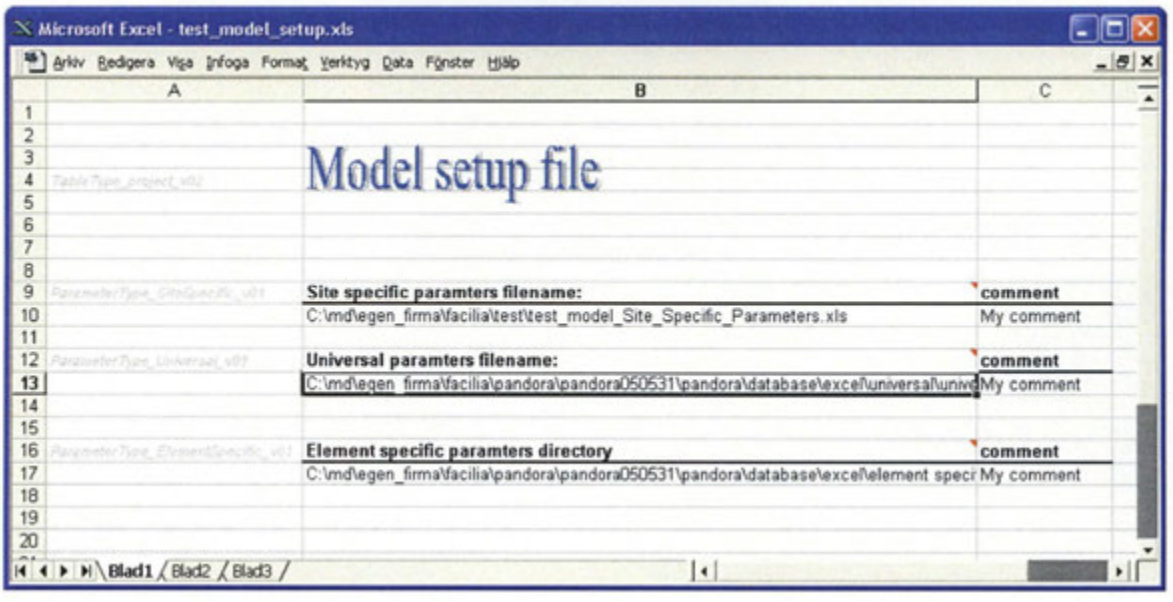

Figure 3.1. *Model set-up file (the main sheet) in Excel.*

In the leftmost column (column A) of the Excel sheet tags can be found. These tags must not be changed.

This sheet must be placed in the same folder as the model, and its name must be: *modelname_setup.xls* where *modelname* is the name of the model. The set-up sheet must contain three fields:

- Site-specific parameters filename (section 3.1.1),
- Element-specific parameters filename (section 3.1.2),
- Universal parameters filename (section 3.1.3).

3.1.1 Site-specific parameters

Site-specific parameters are stored in one Excel sheet per model. An example of such file is shown in figure 3.2.

In the leftmost column (A) of the Excel sheet, a tag can be found (in fig. 3.2, *Table-Type_param_v01*). This tag must not be changed.

New site-specific constants can be added by inserting new rows in the sheet. The new row must be inserted below the tag and above the STOP markers (in fig. 3.2, on line 14).

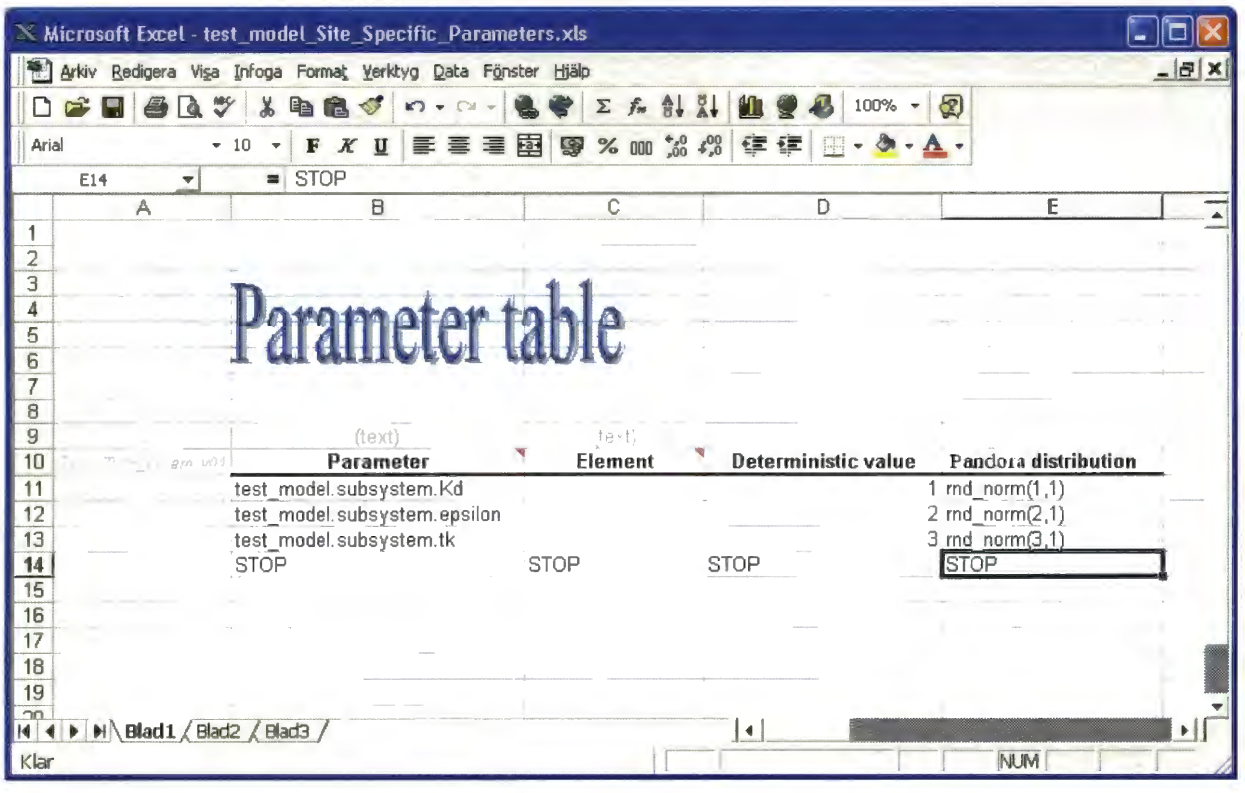

Figure 3.2. *Excel file of the site-specific parameters.*

The properties that can be specified for a parameter are the following:

- Parameter - the actual name of the parameter in Matlab workspace,
- Element - element for which the parameter is valid (if also a nuclide-dependent parameter),
- Deterministic value - the value to be used in deterministic simulations,
- Pandora distribution - distribution to be used in probabilistic simulations.

For a deterministic simulation only *Parameter* and *Deterministic value* have to be specified. For a probabilistic simulation also the Pandora distribution have to be specified.

In Pandora version 1 the following distributions are supported (the Pandora distributions):

- *rnd_uniform(min,max)* - uniform distribution
- *rnd_triang(min,mode,max)* - triangular distribution
- *rnd_logtriang(min,mode,max)* - logtriangular distribution
- *rnd_norm(mu,sigma)* - normal distribution
- *rnd_lognorm(mu,sigma)* - lognormal distribution

There is also a possibility to add other properties for the parameter in the Excel sheet for information to the reader (e.g. Unit, Literature references etc.). Pandora will ignore such properties.

3.1.2 Element-specific parameters

Element-specific (or nuclide- or species-dependent) parameters are stored in one Excel sheet per parameter, all files stored in the same directory. An example of an Excel file for an element-specific parameter is shown in figure 3.3.

The properties that must be specified for an element-specific parameter are:

- Parameter - the actual name of the parameter in the Matlab workspace,
- Element - element for which the parameter is valid,
- Deterministic value - value to be used in deterministic simulations,
- Pandora distribution - distribution to be used in probabilistic simulations.

In figure 3.3, a part of an excel sheet for an element-specific parameter called Kd_peat is shown. In addition to the four mandatory properties above, this sheet has a number of optional parameters for information to the user.

Note that for the element-specific constants one Excel sheet is needed for each parameter, and the name of the Excel file must start with the parameter name. In the example of figure 3.3 the name of the parameter is KD_peat and thus KD_peat_R0228.xls is a valid name for the Excel sheet, the rest of the file name indicating supplementary information for the user. All Excel sheets for Element specific parameters must be stored in the same directory on the file system.

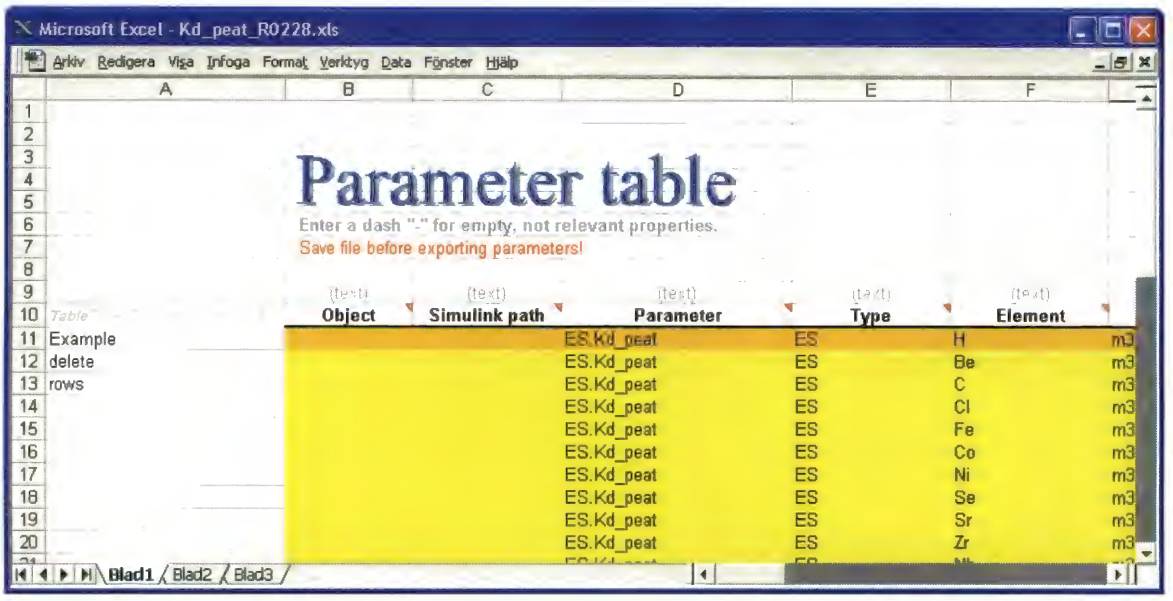

Figure 3.3. *An Excel file for an element-specific parameter.*

3.1.3 Universal parameters

Universal parameters, such as physical constants, are all stored in one Excel sheet. An example of such a file is shown in figure 3.4.

The parameter properties that must be specified in the sheet for the universal constants are the same as for site-specific parameters (section 3.1.3).

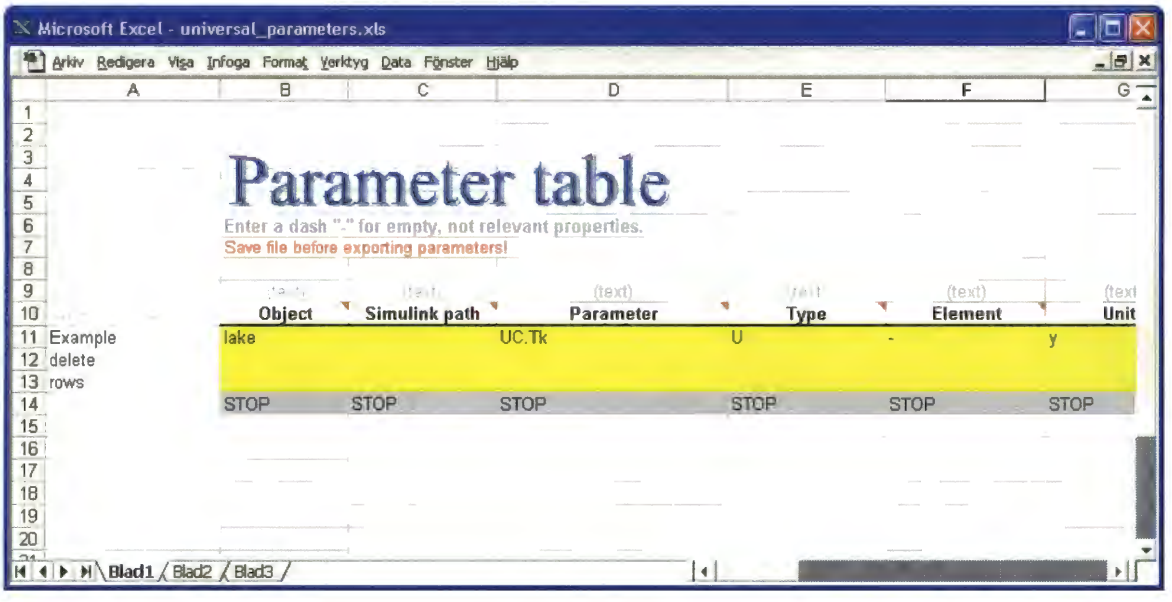

Figure 3.4. *Excel file for the universal parameters.*

3.2 Parameter Editor

During development of models a simplified parameter handling is possible. This is done with the Parameter Editor (figure 3.5). This dialogue[a] has a separate view for Universal, Element Specific and Site Specific parameters.

The Parameter Editor is complement to the Excel sheet approach for users who prefer not to use the sheets directly. At any time it is possible to put the parameters into Excel sheets instead as described here.

The Parameter Editor shows the current deterministic values, units and distributions of the parameters and allows editing directly in the table shown. Parameters not yet defined are marked *NaN* (Not a Number) in the table. The Parameter Editor saves parameters locally in the Radionuclide Manager block (section 4.1) so parameters are automatically saved with the model.

3.3 Pandora Manager

The Pandora Manager (figures 3.6 to 3.15) is a graphical user interface implemented to facilitate the following functionality: Parameter report settings, subsystem editing, function editing, editing of the radionuclide and filter blocks and control of the launch of probabilistic simulation runs.

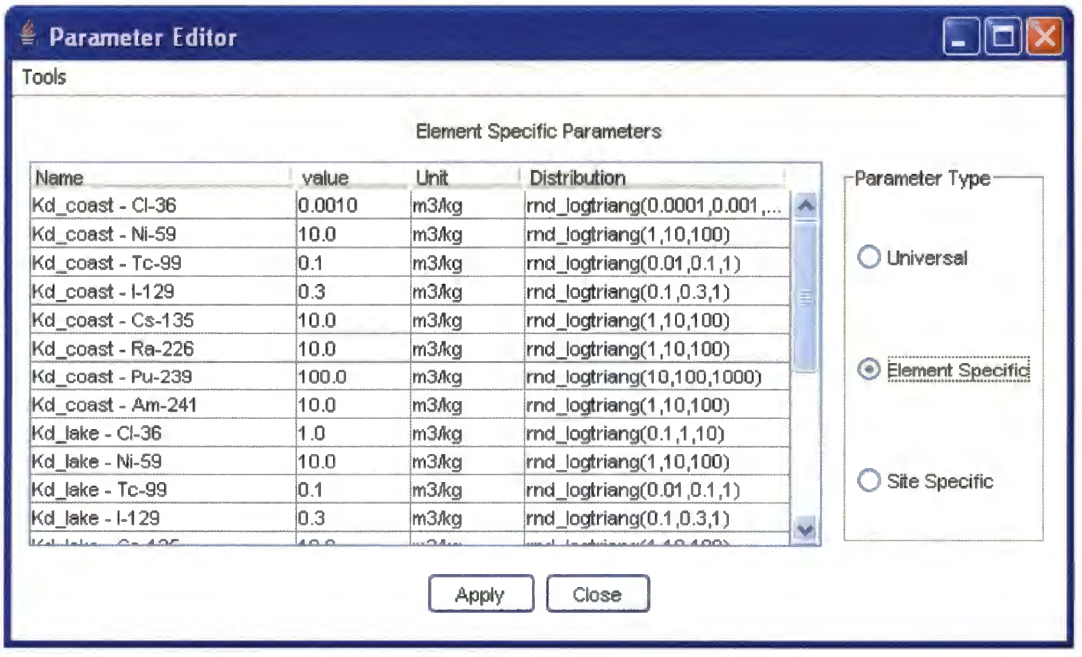

Figure 3.5. *Example view of the Parameter Editor dialogue.*

[a] To open, press button *Edit parameters* in the *Parameters* tab in the Pandora Manager, see section 3.3, or choose from the menu *Tools* > *Edit parameters*.

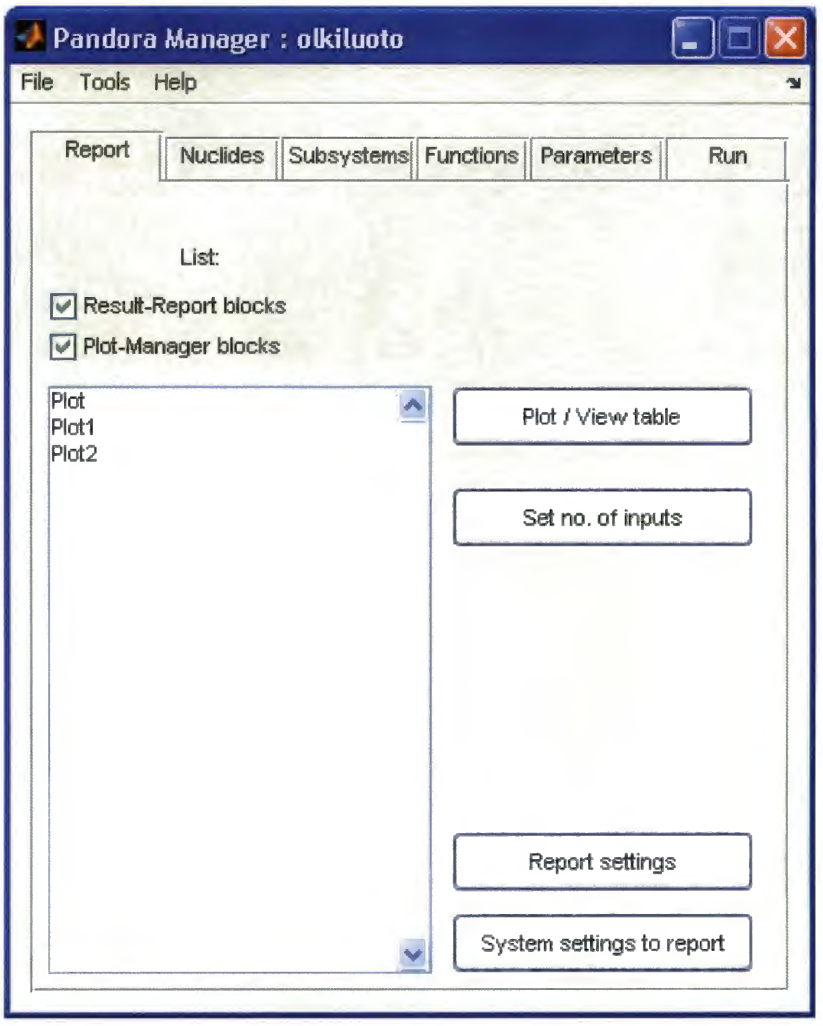

Figure 3.6. *The Report tab of the Pandora Manager.*

The Pandora Manager has three menus that are always visible:

- *File* menu containing:
  - *New Model* - to create a new model,
  - *Open Model* - to open an existing model,
  - *Save Model* - to save the current model,
  - *Save parameters* - to save the parameters and nuclide information (selected nuclides and decay chains) to a separate file,
  - *Load parameters* - to load previously saved parameters.
- *Tools* menu containing:
  - *List Equations* - shows a list of the differential equations represented by the model,
  - *Open project file* - opens the main Excel set-up sheet with links to the parameter files (figure 3.1),
  - *Import project file* - opens a file selection dialogue to import a project file from another project or elsewhere on the file system,

  - *Load params from Excel* - load the parameter values defined in the Excel sheets (sections 3.1.1 to 3.1.3),
  - *Export Nuclide Chain to .xls file* - to export nuclide chains to an Excel file,
  - *Import Nuclide Chain from .xls file* - to import a chain from an Excel file,
  - *Clear Cache* - clears the intermediate Matlab files created from the Excel sheets; this is normally not necessary since the intermediate files are updated automatically when an Excel file is changed,
  - *Create Excel templates for undefined parameters* - creates automatically a template for the parameter file and for files of the site-specific parameters (for a newly created model),
  - *Edit parameters* - opens the Parameter Editor (figure 3.5) for local editing of parameters.
- *Help* menu containing:
  - *User Guide* - opens the Pandora User Guide,
  - *About* - gives some information about Pandora version currently used.

In addition to the menus, the Pandora Manager user interface has the following six tabs discussed in detail below: *Report*, *Nuclides*, *Subsystems*, *Functions*, *Parameters*, and *Run*.

3.3.1 Report tab

In the *Report* tab (figure 3.6) the controls for reporting the results are located. In the list box to the left, the blocks supporting the Plot block (section 4.6) and the Result Report blocks (section 4.5) are listed. By double-clicking one of the items in the list box the corresponding user interface for the block is opened.

On the right side of the *Report* tab, the following pushbuttons are located:

- *Plot / View table* - shows a plot from a Plot block or opens a table with the results in Excel,
- *Set no. of inputs* - sets the number of inputs of a Plot or Result Report block,
- *Report settings* - opens the mask for the Parameter Report block in the model (described in detail in section 4.5),
- *System settings to report* - allows selection of the simulation settings to be reported (described in detail in section 4.5).

3.3.2 Nuclides tab

The *Nuclides* tab (figure 3.7) of the Pandora Manager controls the nuclides in the model. As with the parameters (section 3.1), also the handling of the nuclide information is based on Excel sheets with partial complementary handling options through the user interface of the Pandora Manager. In the list box to the left of the dialogue the nuclides present in the model, and their half-lives in years are shown.

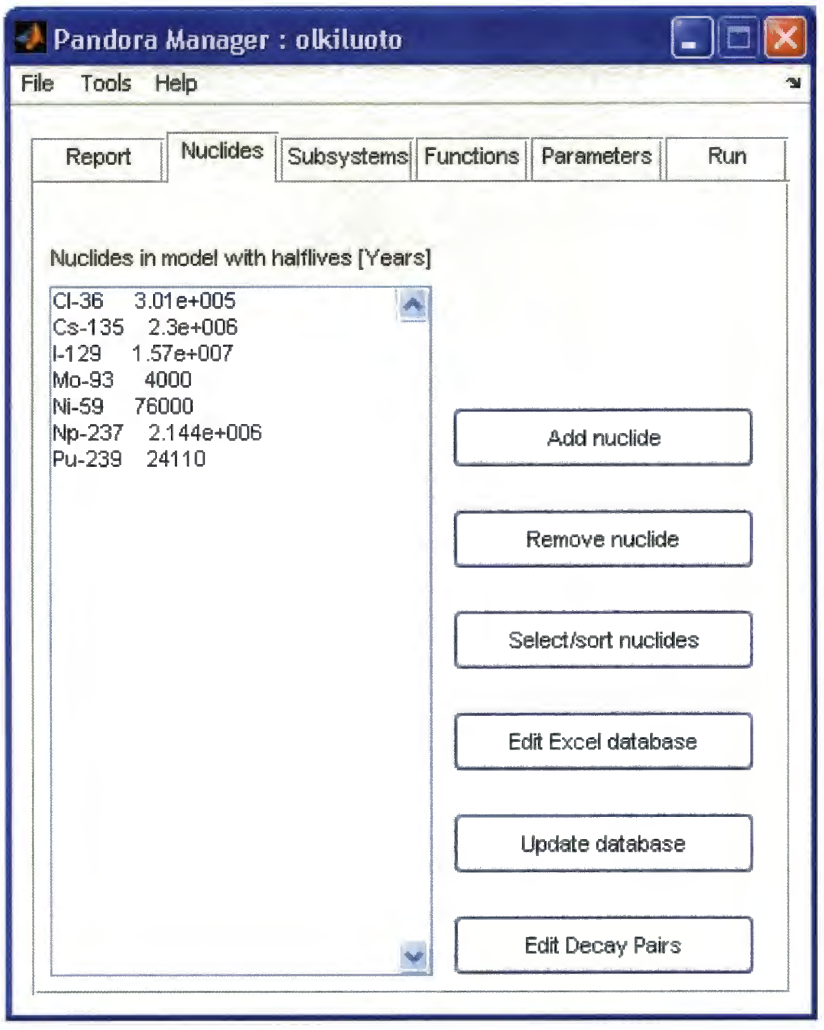

Figure 3.7. *The Nuclides tab of the Pandora Manager.*

The *Nuclides* tab has six pushbuttons:

- *Add Nuclide* - opens a dialogue to add a nuclide to the model,
- *Remove nuclide* - opens a dialogue to remove a nuclide from the model,
- *Select/sort nuclides* - opens a dialogue to change the order of the nuclides in the model and in the reports,
- *Edit Excel database* - opens the Excel sheet containing the nuclide information (see below),
- *Update database* - synchronises the nuclide information between the Pandora Manager and the Excel sheet containing the nuclide information,
- *Edit Decay Pairs* - opens a dialogue to edit decay chains in the model (see below).

Defining of the nuclide half-lives

The input of half-lives is done in an Excel sheet called *halflifesXXX.xls* (where *XXX* stands for any text) in the Element Specific parameters directory on the file system.

Once the half-lives for a number of nuclides are specified in this file they can be loaded to the model by pressing the *Update database button* in the *Nuclides* tab (figure 3.7). When a nuclide is selected in the model the name of it is stored in the Radionuclide Manager block (section 4.1), and saved with the model.

Handling of decay chains

Decay chains can be defined in the model. This information is saved in the Radionuclide Manager block (section 4.1), and thus saved with the model. There is also a possibility to store the decay chain information externally in Excel sheets, comparable to the model parameter handling (section 3.1).

The Chain Editor in figure 3.8a shows the decay of nuclides into each other by a branching decay for each pair. For example, in the figure, *Nuclide 1* decays both into *Nuclide 2* with branching ratio of 0.3 and into *Nuclide 3* with branching ratio of 0.7. *Nuclide 2* decays further into *Nuclide 4* with a 100% branching ratio.

A new decay pair can be created by pressing the *Add Pair* button of the Chain Editor, resulting a dialogue (figure 3.8b) to appear

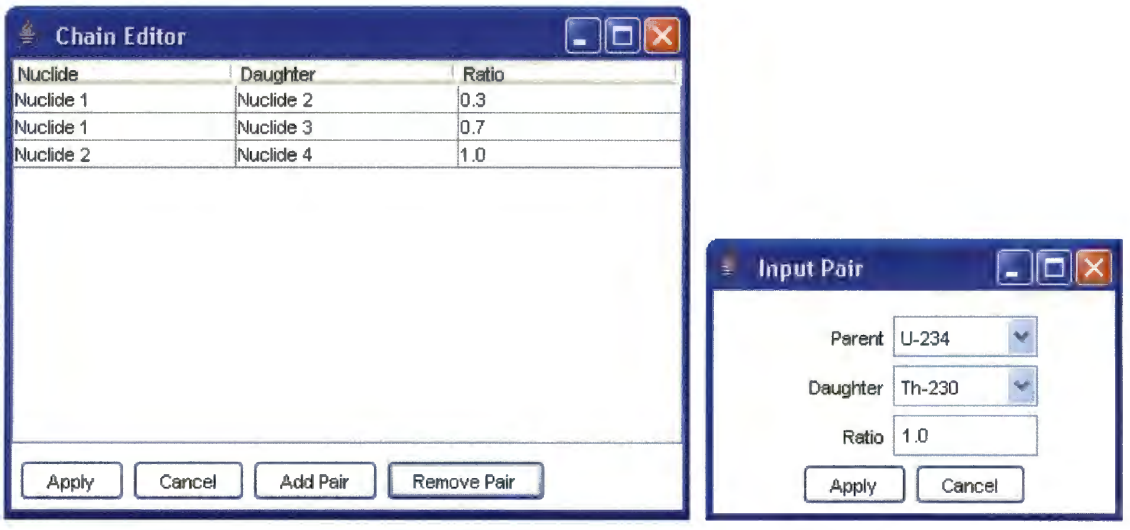

Figure 3.8. a) *The Chain Editor dialogue (left),* ***b)*** *The Input Pair dialogue for adding a decay pair from the Chain Editor (right).*

This Input Pair dialogue contains three fields that select the parent, the daughter and the branching factor for the decay pair. Selection of the parent and the daughter is implemented by using the drop down lists. The branching ratio can be typed as a number between zero and one. The drop down lists contain only the nuclides present in the model; before creating a decay chain, the needed nuclides need to be added to the model. After adding a new pair, the branching ratio can be edited directly in the Chain Editor by double clicking on the ratio field and typing in new branching ratio.

To remove a pair, the decay pair to be removed is selected by clicking any of the fields of the decay pair, and clicking the *Remove Pair* button of the Chain Editor.

3.3.3 Subsystems tab

The *Subsystems* tab (figure 3.9) of the Pandora Manager helps to find and edit the subsystems in the model. In the list box to the left of the dialogue the subsystems in the model are shown. It is also possible to only show the Pandora subsystems with the tick box above the list, resulting in omitting the other (elementary) Simulink blocks from the list. A listed block is shown in the model by clicking its name.

The *Subsystems* tab has the following buttons:

- *Open* - to open the selected subsystem,
- *Remove Image* - to remove an image on the selected block,
- *Set Image* - to set an image on the selected block (for details, see the Simulink documentation on putting an image on a subsystem),
- *Set out-sig. names* - to propagate names of Out ports to connected lines,
- *Terminate outputs* - to terminate unconnected Out ports to avoid warning messages when running simulation,
- *Constant inputs* - to connect a Constant+ block to unconnected In ports; the name of the Constant+ block is taken from the port name,
- *Ground inputs* - to connect a Simulink ground block to unconnected In ports.

For further description of the functions of the *Subsystems* block, see the implementation description of the test in chapter 5.

3.3.4 Functions tab

The *Functions* tab (figure 3.10) of the Pandora Manager lists all the Function blocks (section 4.4) used in the model. The buttons of the tab are:

- *Add input* - adds a new input to the function,
- *Constant inputs* - connects a Constant+ block (section 4.3) to the unconnected In ports (the name of the Constant+ block is taken from the port name),
- *Ground inputs* - connects a Simulink ground block to unconnected In ports.

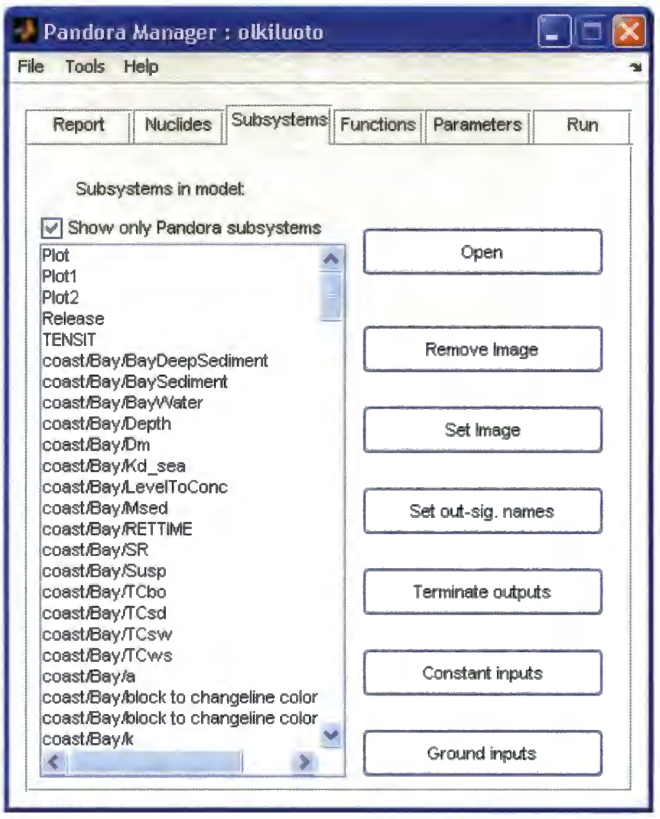

Figure 3.9. *The Subsystems tab of the Pandora Manager.*

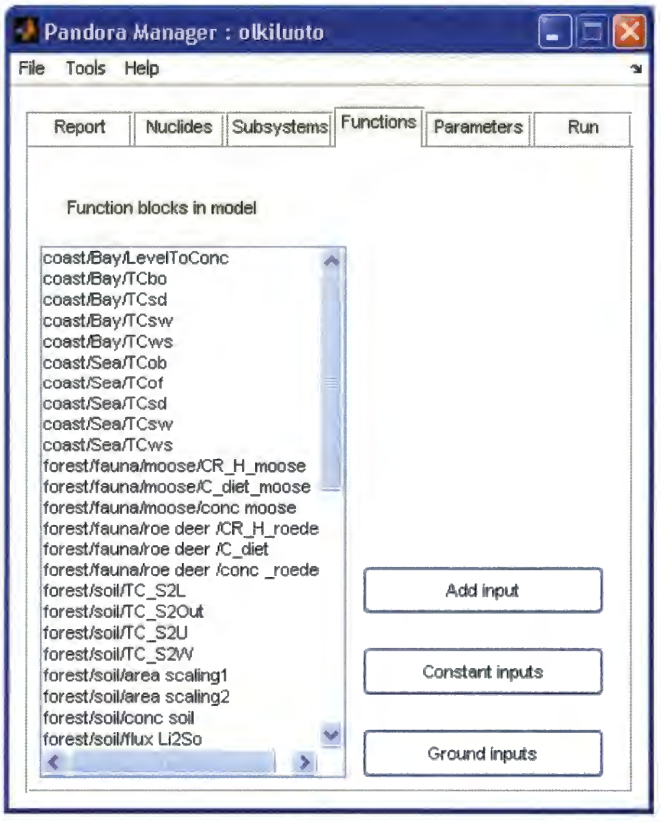

Figure 3.10. *The Functions tab of the Pandora Manager.*

3.3.5 Parameters tab

The *Parameters* tab (see figure 3.11) of the Pandora Manager has two list boxes. The left one lists all Constant+ blocks (section 4.3) in the model and the right one lists the paths to the Excel sheets containing the parameters (section 3.1). The Excel path list box does not update automatically due to the long access time to the sheets; instead there is a button *Refresh filelist* to update the list.

A single click in the left list box will show the corresponding Constant+ block in the model. A double click in the left list box will open the Excel sheet with the corresponding parameter.

A double click in the right list box will lets select new files for the site-specific or universal parameters or a new directory for the element-specific parameter files.

The *Edit parameters* button opens the Parameter Editor described in section 3.2.

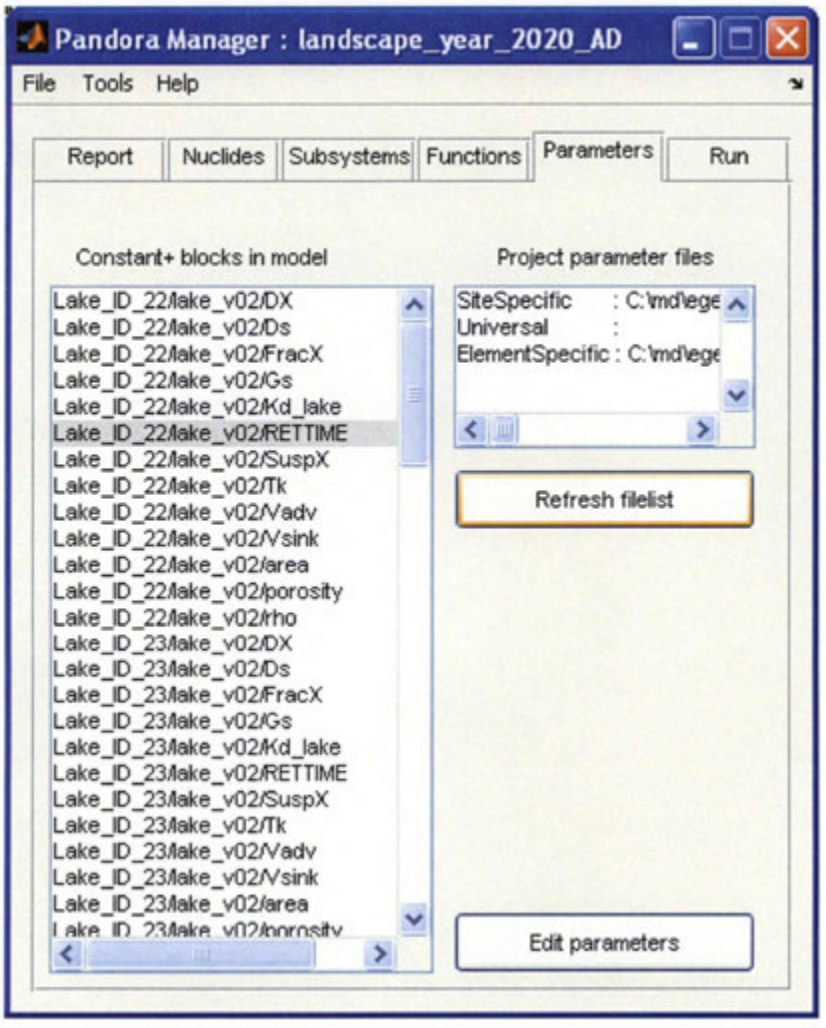

Figure 3.11. *The Parameters tab of the Pandora Manager.*

3.3.6 Run tab

The *Run* tab (figure 3.12) is essentially an interface to the *probsim* script, callable also directly from the Matlab prompt, for running probabilistic simulations.

The settings found on the *Run* tab are the following:

- *Parameters to sample* - lists the parameters of the model to be sampled in the simulation,
- *Select Parameters to sample* - opens a dialog (figure 3.13) for selection of the parameters to sample from the set of parameters present in the model,
- *Random seed type* - a combo-box for choosing between random (time-based) sampling and specified seed; in the latter case a input field is enabled for entering an integer value as seed for the random number generator, and in the former case the seed is created from the current time value read from the computer clock,

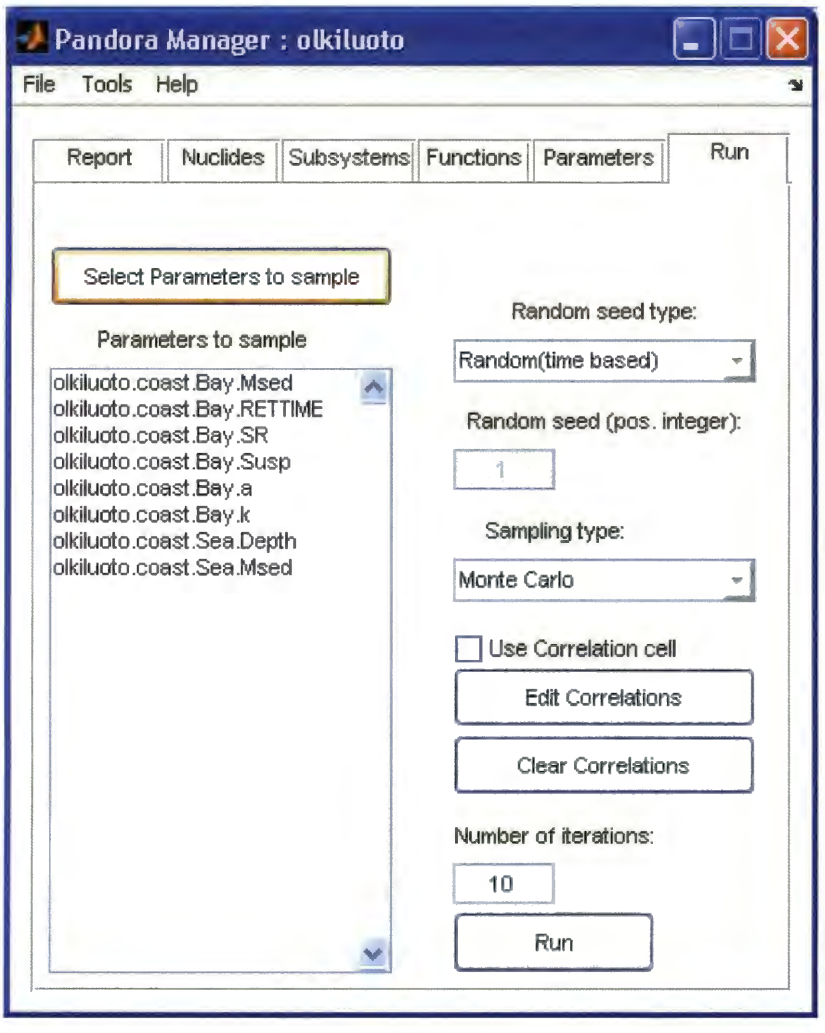

Figure 3.12. *The Run tab of the Pandora Manager.*

- *Sampling type* - a combo-box for choosing between normal Monte Carlo sampling and Latin Hypercube sampling, a method to create the distribution of a parameter in fewer samples than with simple random sampling (see e.g. McKay et al. 1979),
- *Use Correlation cell* - checkbox for enabling specified correlations between the parameters in the simulation; a correlation cell for the *probsim* script has to be created,
- *Edit Correlations* - opens a dialogue (figure 3.14) for selecting parameters to be correlated with each other, or when the parameters to be correlated are selected the Correlations Editor (figure 3.15) is opened with the current correlation cell, specifying the wanted correlation by a value between –1 and 1.

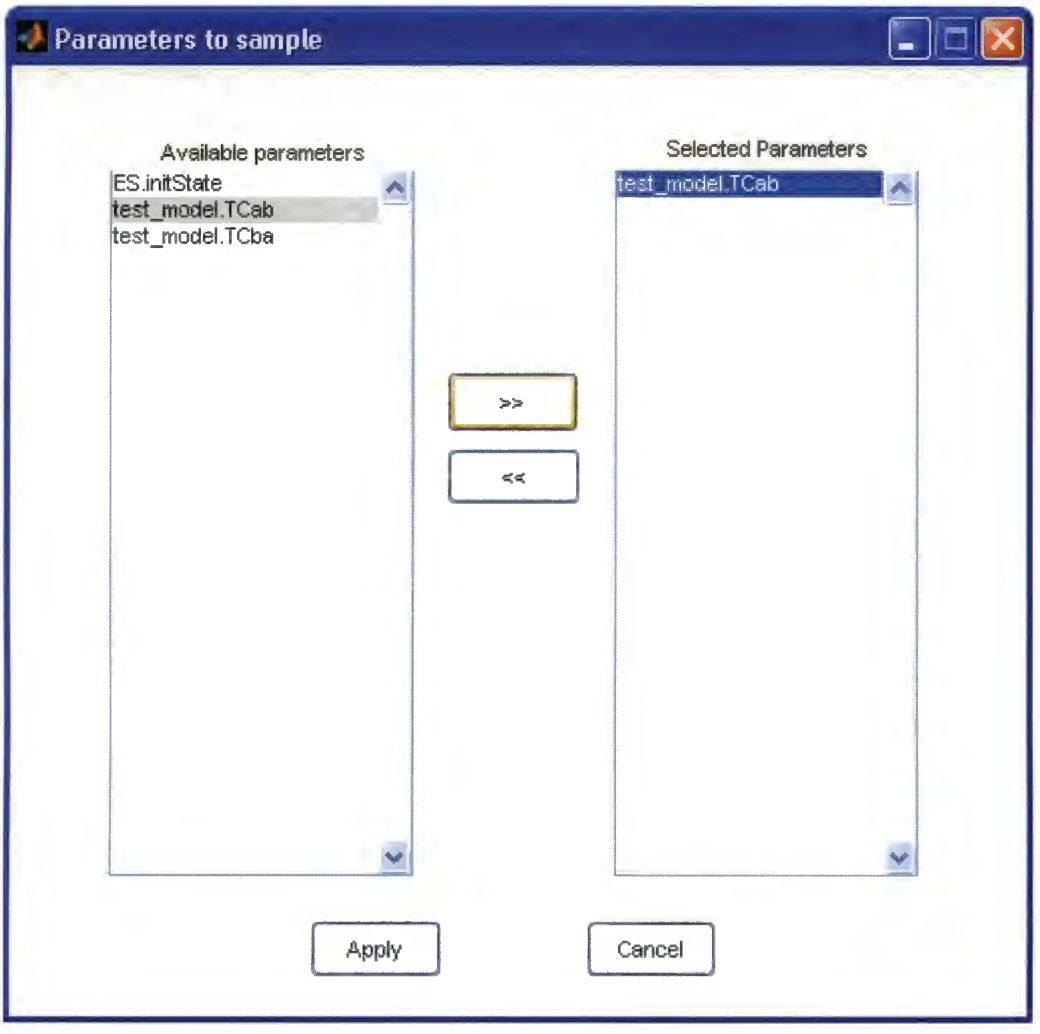

Figure 3.13. *The Parameters to sample dialogue opened from the Run tab of the Pandora Manager by pressing the Select parameters to sample button.*

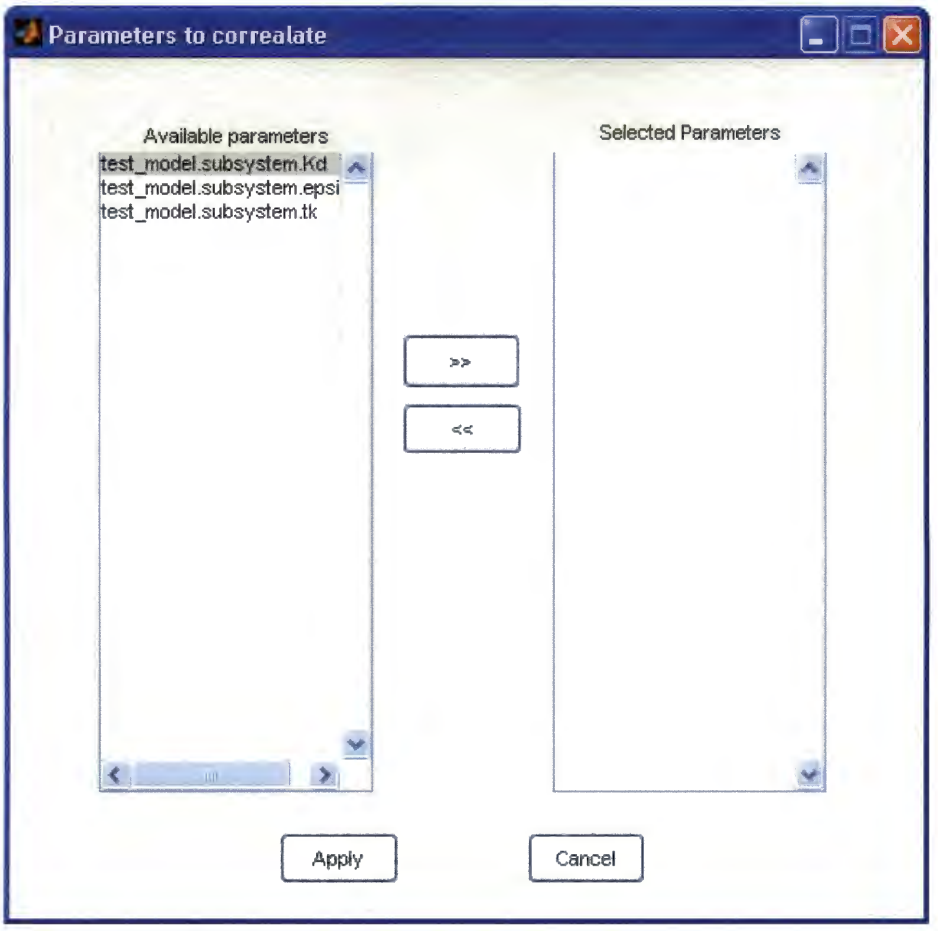

Figure 3.14. *The Parameters to correlate dialogue opened from the Run tab of the Pandora Manager by pressing the Edit correlations button.*

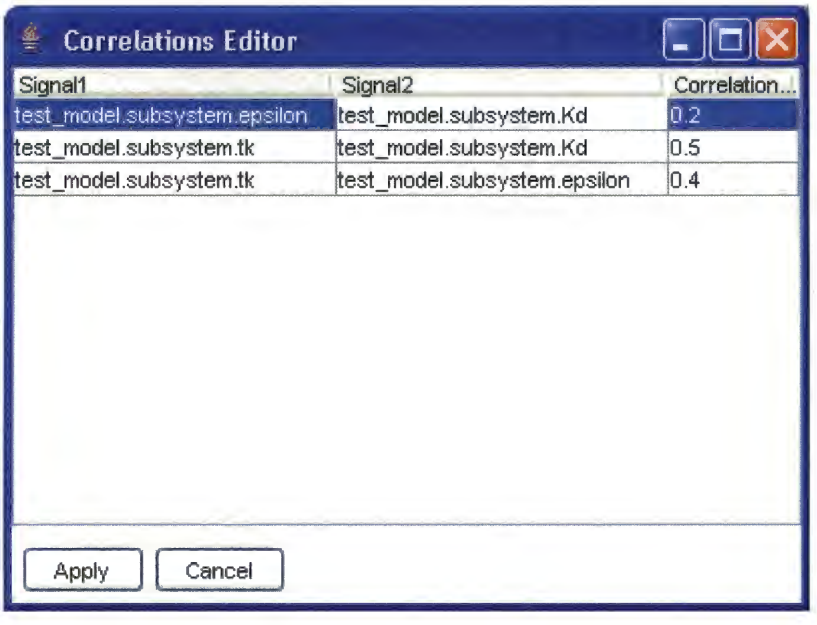

Figure 3.15. *The Correlations Editor dialogue.*

4 PANDORA BLOCK LIBRARY

In this chapter the different specifically created blocks in the Pandora library are described. The Pandora blocks reside in the Simulink library and can be used in the same way as the built-in Simulik blocks after Pandora is installed (App. A). Some of their features can be controlled from the Pandora Manager as described above in chapter 3.

4.1 Radionuclide Manager block

The Radionuclide Manager block (figure 4.1), also known as the Pandora block, allows centralised selection and handling of multiple radionuclides to be included in a Pandora model. The radionuclides to be included in the model are selected and arranged to the desired order. The signals will follow this order in all blocks used in the model. One Radionuclide Manager block is needed in every Pandora model.

In addition to the names of simulated nuclides (or elements or species), the Radionuclide Manager block specifies their half-lives and decay chains in the model (figure 4.1). For stable, non-decaying, materials, using *Inf* (infinite) as half-life is allowed. A zero matrix is to be used as the chain for non-branching decay. These properties can be handled also through the Pandora Manager (section 3.3.2).

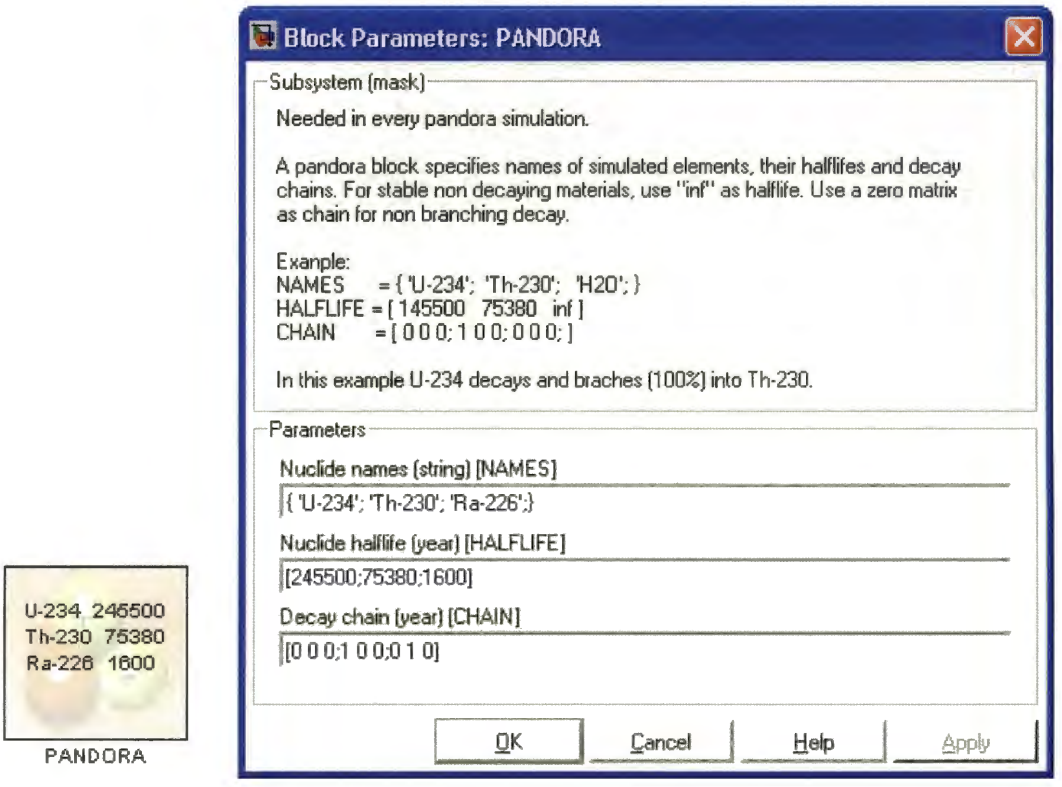
U-234 246500
Th-230 75380
Ra-226 1600
PANDORA
Block Parameters: PANDORA
Subsystem (mask)
Needed in every pandora simulation.
A pandora block specifies names of simulated elements, their halflifes and decay chains. For stable non decaying materials, use "inf" as halflife. Use a zero matrix as chain for non branching decay.
Example:
NAMES = { 'U-234'; 'Th-230'; 'H2O'; }
HALFLIFE = [145500 75380 inf]
CHAIN = [0 0 0; 1 0 0; 0 0 0;]
In this example U-234 decays and braches (100%) into Th-230.
Parameters
Nuclide names (string) [NAMES]
{ 'U-234'; 'Th-230'; 'Ra-226';}
Nuclide halflife (year) [HALFLIFE]
[245500;75380;1600]
Decay chain (year) [CHAIN]
[0 0 0;1 0 0;0 1 0]
OK
Cancel
Help
Apply

Figure 4.1. *The Radionuclide Manager block (left) and its user interface (right).*

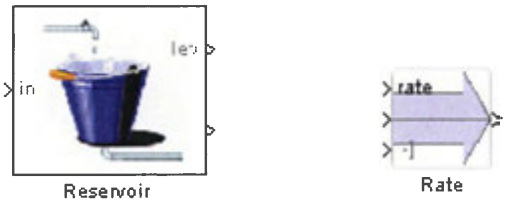

Figure 4.2. *The Reservoir block (left) and the Rate block (right).*

In any Pandora model it is possible to include only one Radionuclide Manager block. When doing this, decay and in-growth data, as well as the names of the selected radionuclides become available throughout the entire model. The names of the radionuclides are not transferred in the model, but are instead read from the Radionuclide Manager. There is, therefore, no need or possibility to connect the Radionuclide Manager block with other blocks in the model.

4.2 Reservoir and Rate blocks

The Reservoir block (figure 4-2) has one In port representing incoming flux to be integrated. The Reservoir block corresponds to a compartment in the classical conceptual transport models. The first Out-port is *level* signalling the current level of integration. The remaining Out ports are flux-out ports. They are designed to be connected only to the Rate block (figure 4-2) controlling the outflow from the Reservoir block.

The Rate block is meant to control outgoing flux from Reservoir blocks. A flux-out port from a Reservoir is connected directly to the centre In port of the Rate block. A signal carrying the transfer rate coefficient (typically from a Function block, see section 4.4) is connected to the *rate* port, and then the outgoing flux of the Reservoir block is controlled by the *rate* signal through a hidden backward connection to the Reservoir block. The Rate block with a given rate corresponds to a transfer (expressed as a transfer coefficient) in the classical conceptual transport models.

The third In port in the Rate block is for symmetry only and can be left unconnected or connected to a Simulink ground block.

The half-life vector (HALFLIFE) and decay matrix (CHAIN) specified in the Radionuclide Manager block are available in the Reservoir block. The decay is calculated according to the formula

$$\frac{dY}{dt} = C \cdot Y\lambda - Y\lambda \qquad (4.1)$$

where Y is the vector of nuclide levels, C is the CHAIN matrix, λ is ln(2)/HALFLIFE, and $Y\lambda$ denotes element wise multiplication of Y and λ.

a) b)

Figure 4.3. a) *The three variants of the Constant+ block corresponding to the site-specific, element-specific and universal parameters.* ***b)*** *The Function block.*

4.3 Constant+ blocks

The Constant+ block (figure 4.3a) has three variants representing the site-specific, element-specific and universal parameters (cf. section 3.1). The site-specific and universal variants are intended for scalar parameters and the element-specific for vector (nuclide-dependent) input.

The block searches after a Matlab workspace variable name to obtain its data. The variable names are constructed differently depending on the three modes, or variants:

- Site-specific mode: the parameter has a name such as coast/bay/depth, and all slashes (/) are replaced by dots (.) to give the structured variable name: coast.bay.depth,
- Universal mode: the parameter has a name such as coast/bay/g, and the last part of the name is taken and a prefix *UC.* is added giving the variable name UC.g,
- Element-specific mode: the parameter has a name such as coast/bay/Kd, and the last part of the name is taken and a prefix *ES.* is added giving the variable name ES.Kd.

4.4 Function block

The Function block (figure 4.3b) translates an expression string given in the block dialogue (figure 4.4) to the elementary Simulink blocks like in the example of figure 4.5. The mathematical operations of Table 4.1 are supported by the block. The function is also editable through the dialogue.

4.5 Result Report and Parameter Report blocks

The reporting blocks are used in connection with the Pandora Manager to control the generation of reports on simulation results and parameters.

The Results Report block exports named numerical data generated during a simulation to text files or to an Excel worksheet. From the interface of this block (figure 4.7), the time range that will be exported is selected. Data from any Simulink block in the model can be exported to text files or Excel (by connecting it to the Excel Link Manager block).

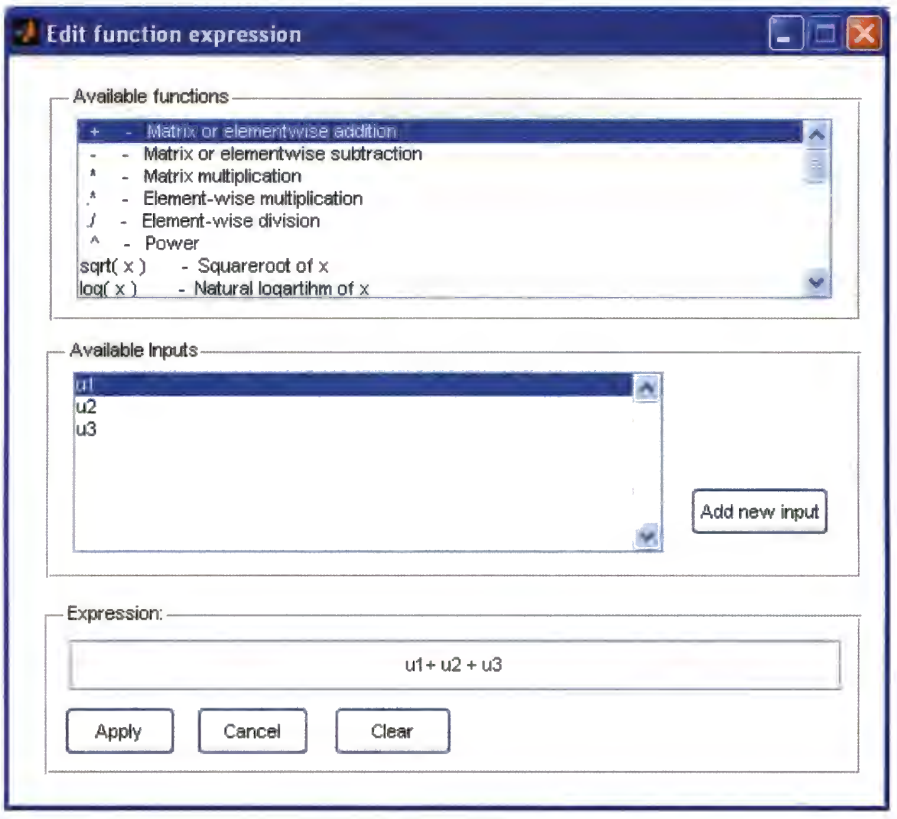

Figure 4.4. *The Function block dialogue.*

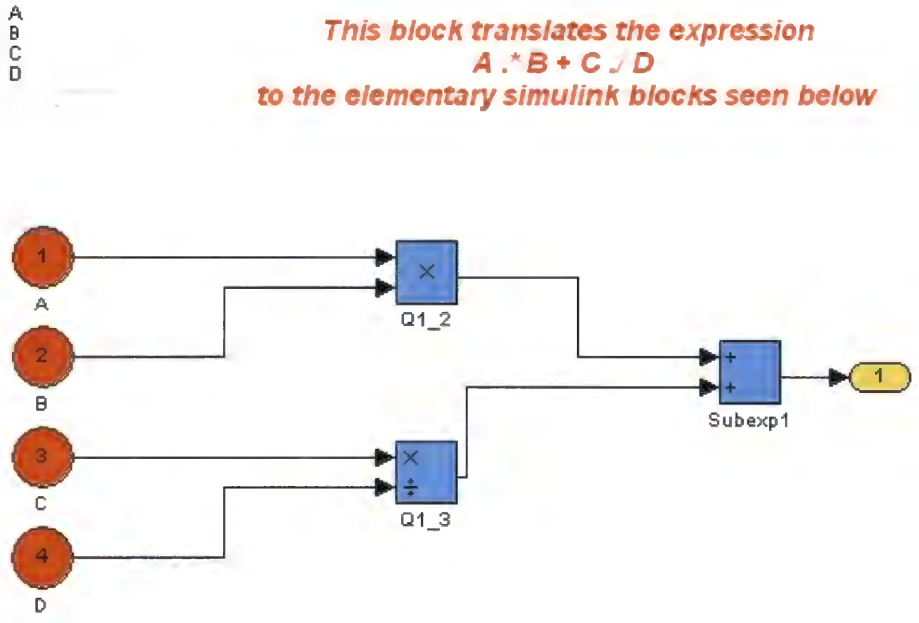

Figure 4.5. *Example of the system of elementary Simulink blocks created by the Function block.*

Table 4.1. *Mathematical operations supported by the Function block.*

Operator/Function	Explanation
+	Matrix or element-wise addition
-	Matrix or element-wise subtraction
*	Matrix multiplication
.*	Element-wise multiplication
./	Element-wise division
^	Power
sqrt(x)	Squareroot of x
log(x)	Natural logarithm of x
log10(x)	Base 10 logarithm of x
transpose(x)	Transpose
inv(x)	Inverse
exp(x)	Exponent
abs(x)	Absolute value
rem(x,y) & mod(x,y)	Remainder and modulus
<,>,<=,>=,==,~=	Relational operations
sign(x)	Signum function
delay(x,y)	Delay x with y time-steps
matsum(x)	Sum the rows of matrix x (returns vector)
floor(x),ceil(x),round(x),fix(x)	Rounding functions

Figure 4.6. *Result Report block (left) and Parameter Report block (right).*

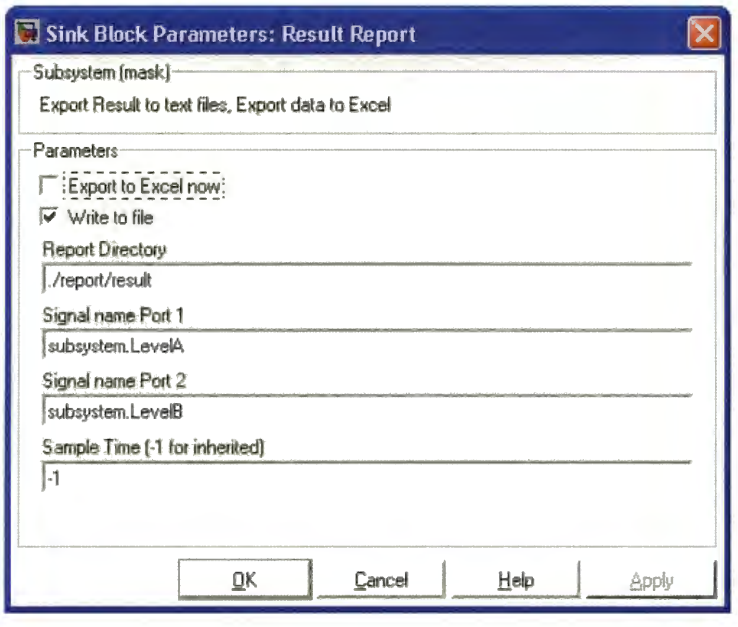

Figure 4.7. *The Result Report block interface.*

The result-report block user interface (figure 4.7) has the following settings:

- *Export to Excel now* - used at any time after a simulation has been run to list the simulation results in Excel,
- *Write to file* - to choose if the results are written to a text file (normally set on when doing probabilistic simulations generating several result files),
- *Report Directory* - to set the report directory,
- *Signal name port [x]* - sets the name to be used in the report for a certain signal; this name is overridden by a name on the signal itself if a signal name is set,
- *Sample time* - sets the interval of reported values, normally set to -1 for inherited, see the Matlab documentation for to-workspace block for further details.

The System Settings Report interface (figure 4.8) is a part of the Parameter Report manager/block available from the Pandora Manager button *System settings to report*. The left list box shows all the available system settings, and the right one the settings selected by user to be reported (by pressing the >> button). The default settings selected automatically are shown in figure 4.8.

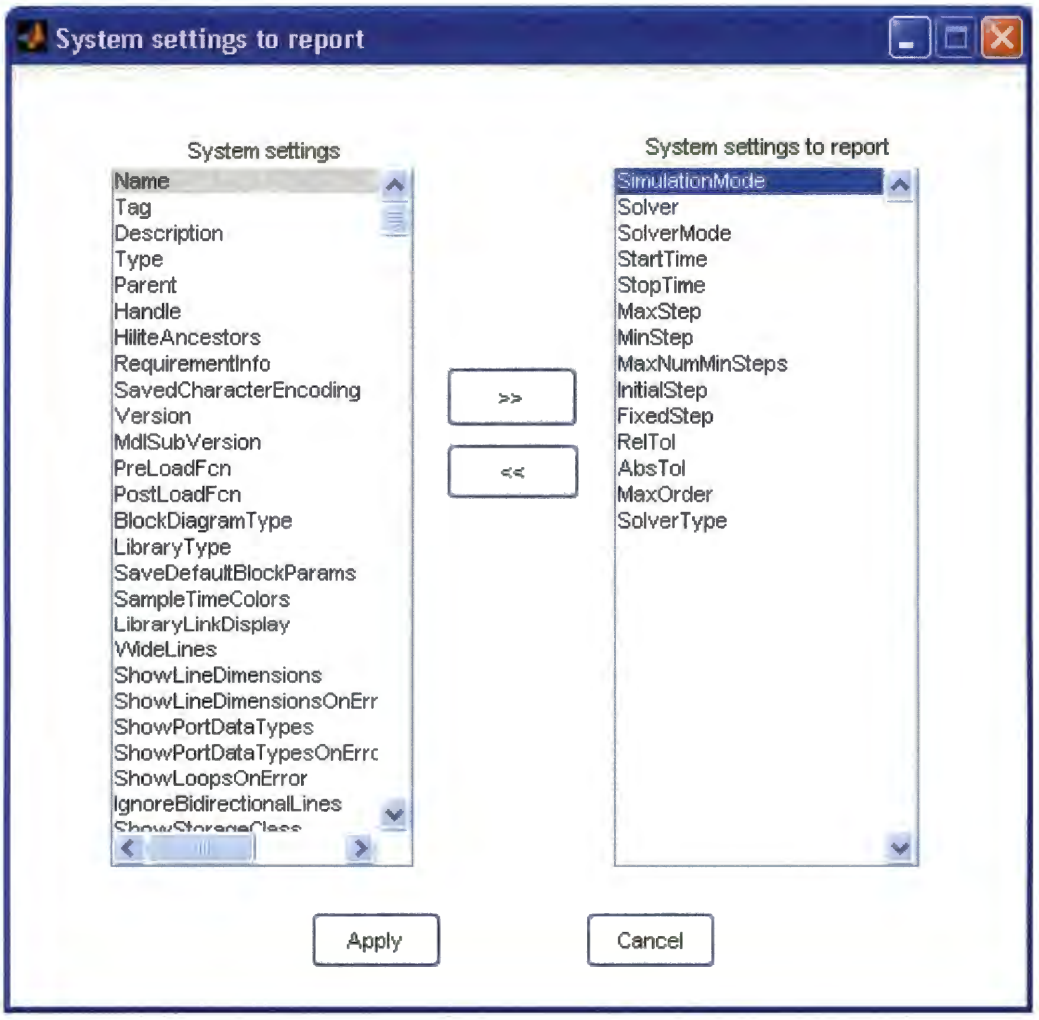

Figure 4.8. *The System Settings Report interface of the Parameter Report block with the default selection.*

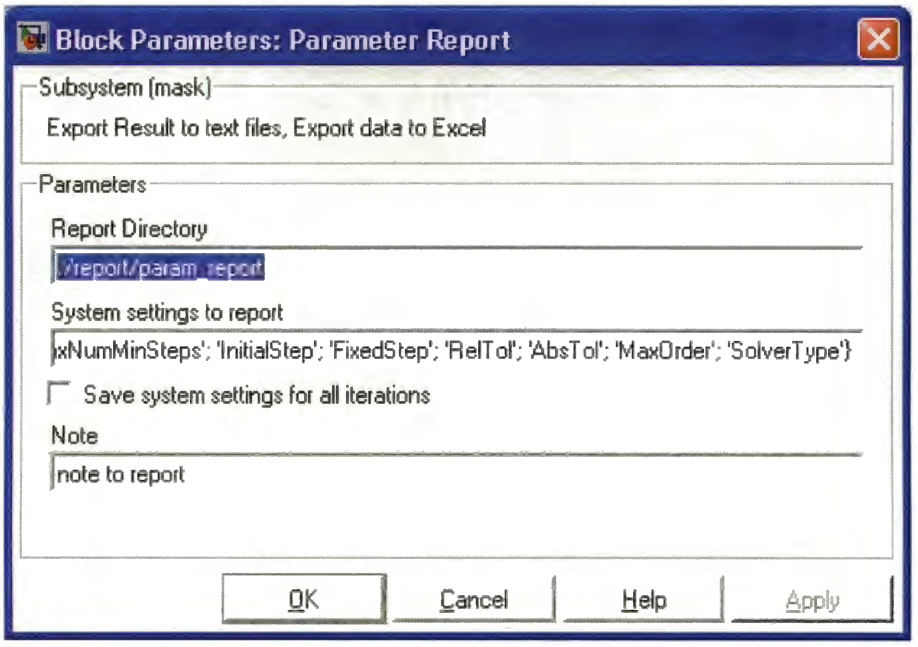

Figure 4.9. *The dialogue available through the Report settings button in the Pandora Manager.*

An additional user interface (figure 4.9) for Parameter Report manager/block is available from the Pandora Manager button *Report settings*. Here the directory for the report can be selected, the field *System settings to report* shows the settings made through the System Settings Report interface, and the checkbox *Save system settings for all iterations* is used to set if the report is written for all iterations in a Monte-Carlo simulation. The field *Note* allows input of a short note to be saved with each report.

4.6 Plot block

The Plot block (figure 4.10) functions in the same way as the Result Report block, but instead of exporting data to text or Excel, it plots the connected signals in a Matlab plot figure. The Plot block also enables the control of line types, legend names etc.

The Plot block interface (figure 4.10) has the following settings:

- *Plot now* - to be used at any time after a simulation is run to draw a plot,
- *Title* - a field to set the plot title.
- *Y-lable* - a field to set the label and unit for the Y-axis, typically Activity [Bq],
- *X-lable* - a field to set the label and unit for the X-axis, typically Time [years],
- *Signal name port [x]* - sets the name to be used in the legend for a certain signal; this name is overridden by a name on the signal itself if a signal name is set,
- *Automatically plot after simulation* - used to choose automatic plotting after each simulation run,
- *Log scales* - sets logarithmic scales in plots,
- *Plot line-styles* - selects the plot line style presented as in Matlab, see the Matlab reference manual for details,

- *Plot colours* - selects the plot line colours presented as in Matlab, see the Matlab reference manual for details,
- *Plot markers* - selects the plot line markers at each time step presented as in Matlab, see Matlab reference manual for details,
- *Sample time* - sets the interval of plot points, normally set to -1 for inherited, see Matlab documentation for to-workspace block for further details.

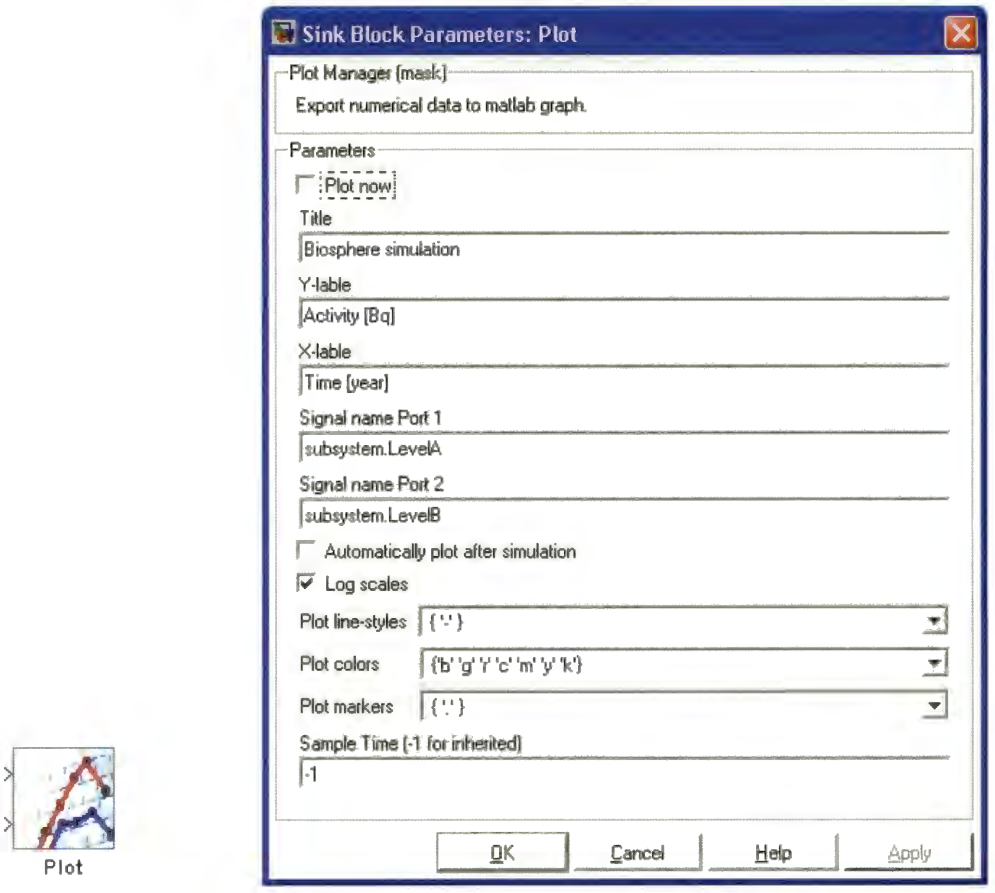

Figure 4.10. *The Plot block (left) and its user interface (right).*

Figure 4.11. *The Filter block (left) and the Selector block (right).*

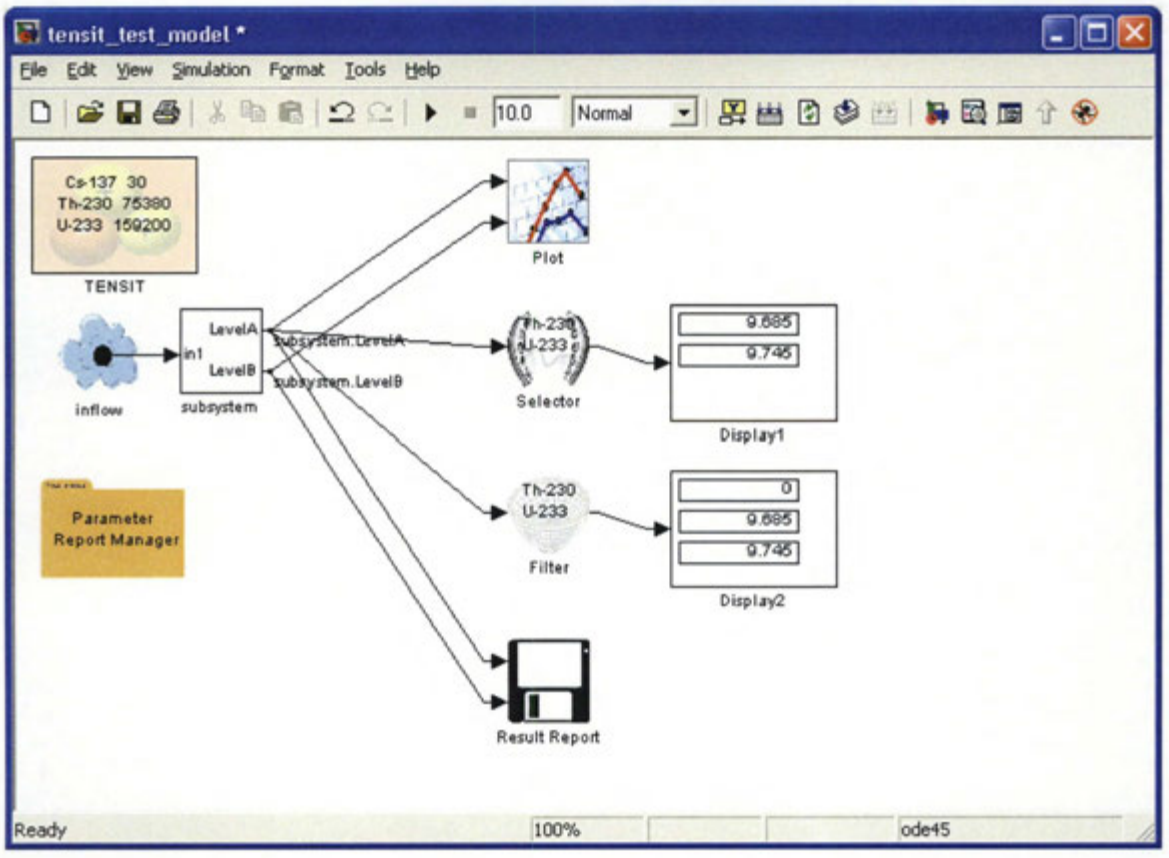

Figure 4.12. *Example of the use of Filter and Selector blocks.*

4.7 Filter and Selector blocks

The Filter block simplifies the implementation of models with different transfer functions for different nuclides, by setting the value of the unwanted nuclides to zero. The Selector block is similar to the Filter block but the unwanted nuclides are removed totally from the signal vector, thus the signal dimension is reduced in a selector. Note that Pandora cannot keep track of the nuclide names after a Selector block, this is up to the user.

The example in figure 4.12 illustrates the use of filter and selector: For *Display1* we have used a selector and thus we have reduced the dimensionality of the signal vector to hold only the selected signals. The use of the filter block is illustrated with *Display2* showing that the dimensionality of the signal vector is preserved and the values for the unselected nuclides are set to zero.

4.8 Unit conversion blocks

The unit conversion blocks (*bq2mole* and *mole2bq*) provide conversion from activity in Becquerel to amount of substance in mole and vice versa, according to the equations

$$Mole = \frac{Bq \cdot HALFLIFE \cdot 60 \cdot 60 \cdot 24 \cdot 365}{\ln(2) \cdot N_A} \tag{4.2}$$

$$Bq = \frac{Mole \cdot N_A \cdot \ln(2)}{HALFLIFE \cdot 60 \cdot 60 \cdot 24 \cdot 365} \tag{4.3}$$

where HALFLIFE is taken from the Radionuclide Manager block and N_A is the Avogadro's number (6.022×10^{23}).

4.9 Block to change line colour

To make the models more readable and aesthetic it is helpful to distinguish lines that represent flux of substance from lines that carry other information. The block to changes the colour of a line from black to grey. Connect the block to any line and the output line colour will be grey. The block does not change the signal in any way; the output equals input.

4.10 Inflow block

The Inflow block has two variants: expression and port modes (figure 4.13a-b). These two blocks can be used to produce an input of nuclides to the system. The size of the input vector will be the same as the number of nuclides in the model.

The expression mode of the Inflow block takes a Matlab expression in its mask dialogue to define its value. The port mode of the Inflow block takes its value from a signal on the In port (typically from an element-specific Constant+ block).

4.11 Statistics block

When a probabilistic simulation is run, statistics is automatically calculated for all Resevoir blocks. The Statistics block (figure 4.13c) is used to define additional statistics nodes in probabilistic simulation. The Statistics block is connected to signals where statistics is to be computed. When probabilistic simulation is run, statistics is automatically calculated for these signals.

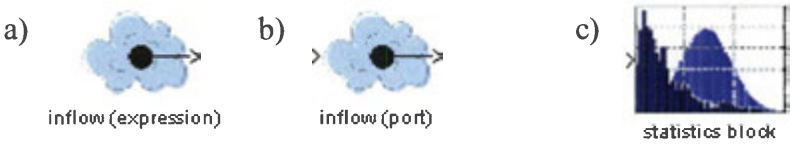

Figure 4.12. a) *Expression mode of the Inflow block.* ***b)*** *Port mode of the Inflow block.* ***c)*** *Statistics block.*

5 EXAMPLE MODEL IMPLEMENTED

As an introduction to using of Pandora, a test model is implemented. Section 5.1 describes the theoretical background of the test model, and section 5.2 gives the practical details of how to implement the model in Pandora.

5.1 Test Case Model

The Test Case model is based on the coast model described in Karlsson et al. (2000) and Bergström et al. (1999). The coast is modelled with six compartments as shown in the conceptual model in Figure 5.1 and system of equations 5.1. The default parameter values for the test use are given in Tables 5.1 and 5.2.

The system of equations defining the mathematical representation of the test case models is

$$\begin{cases} \frac{d(WaterIC)}{dt} = Inflow + TC_{sw} * SedIC + TC_{oi} * WaterOC - TC_{io} * WaterIC - TC_{ws} * WaterIC \\ \frac{d(SedIC)}{dt} = TC_{ws} * WaterIC - TC_{sw} * SedIC - TC_{sd} * SedIC \\ \frac{d(DeepSedIC)}{dt} = TC_{sd} * SedIC \\ \frac{d(WaterOC)}{dt} = TC_{io} * WaterIC + TC_{sw} * SedIC - TC_{oi} * WaterOC - TC_{ws} * WaterOC \\ \frac{d(SedOC)}{dt} = TC_{ws} * WaterOC - TC_{sw} * SedOC \\ \frac{d(DeepSedOC)}{dt} = TC_{sd} * SedOC \end{cases} \quad (5.1)$$

where

$$TC_{io} = \frac{365}{RETTIME} \quad (5.2)$$

$$TC_{sd} = \frac{SR}{Msed} - TC_{sw} \quad (5.3)$$

$$TC_{ws} = \frac{K_d \cdot SR}{D \cdot (1 + K_d \cdot Susp)} \quad (5.4)$$

$$TC_{oi} = \frac{365}{RETTIME} \cdot \frac{V_b}{V_o} \quad (5.5)$$

$$TC_{sw} = RESUSP \quad (5.6)$$

$$TC_{out} = OUTFLOW \quad (5.7)$$

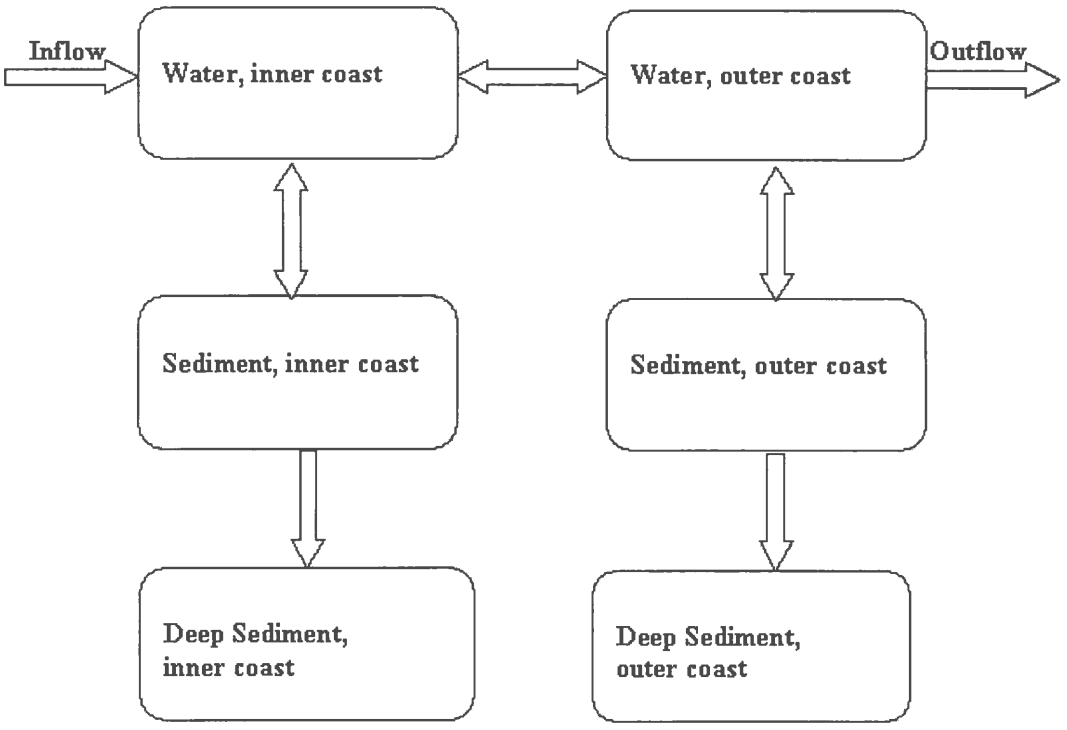

Figure 5.1. *Conceptual representation of the test case model.*

Table 5.1. *Site-specific parameter default values for the test case model.*

Description	Symbol	Deterministic value	Unit
Area of surface, bay	a	1.4e6	m^2
Mean depth, bay	D	2.3	m
Mean residence time of water in bay	RETTIME	45	days
Volume open seacoast box	V_o	1.7e8	m^3
Mean depth, open sea	D	7	m
Sedimentation rate, bay	SR	2.0	kg/(m^2*year)
Sedimentation rate, sea	SR	0.2	kg/(m^2*year)
Suspended matter, bay	Susp	0.001	kg/m^3
Suspended matter, sea	Susp	0.001	kg/m^3
Mass of top sediment	Msed	10	kg/m^2
Resuspension rate from sediment	RESUSP	0.2	$year^{-1}$
Outflow rate, sea	OUTFLOW	44	$year^{-1}$

Table 5.2. *Element-specific parameter default values for Kd of sea sediments (Kd_sea) in the test case model.*

Cl-36	Cs-135	I-129	Mo-93	Ni-59	Np-237	Pu-239
0.001	10	0.3	0.001	10	10	100

5.2 Pandora implementation of test case model

In this section the test model of section 5.1 is implemented in Pandora step by step. We assume that the user is familiar with the basics of Matlab/Simulink. Finally, the implemented model of the coast will correspond to figure 5.1

The instructions are given on this page, and the corresponding figures on the following ones.

1. Start the Pandora Manager by typing *pandora* at the Matlab command prompt (figure 5.2).
2. Open a new Simulink model and name it *coast*.
3. Open the Simulink library browser.
4. Select the Pandora library.
5. Create a subsystem *Inner coast* and add blocks and connections according to figure 5.3.
6. Create a subsystem *Outer coast* and add a blocks according to figure 5.4. Note, that you can also copy it partly from the *Inner coast* subsystem.
7. Connect the two subsystems according to figure 5.5 and add a Radionuclide Manager block, an Element-specific Constant+ block for inflow and a Plot block.
8. Use the Pandora Manager to set the number of inputs on the Plot block by selecting the block either directly in the model or in the list box in the Manager, and then pressing the *Set no. of inputs* button and set the number of inputs to 2.
9. Input the parameter values by pressing the *Edit parameters locally* button in the *Parameters* tab in the Manager. Put in element-specific and site-specific parameter values according to figures 5.6 and 5.7.
10. Select the *Configuration parameters...* settings from the *Simulation* menu in Simulink as in figure 5.8.
11. Run the model.
12. When simulation is ready the plot in figure 5.9 should be shown:

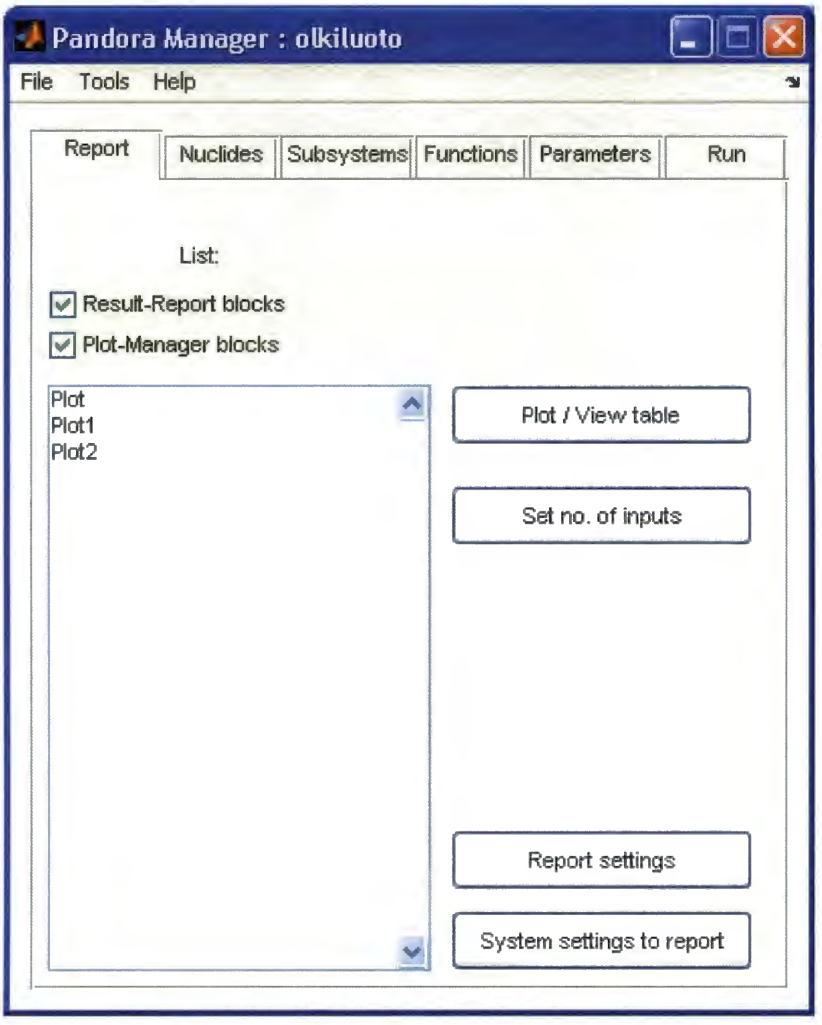

Figure 5.2. *Step 1 of the implementation of the test case model.*

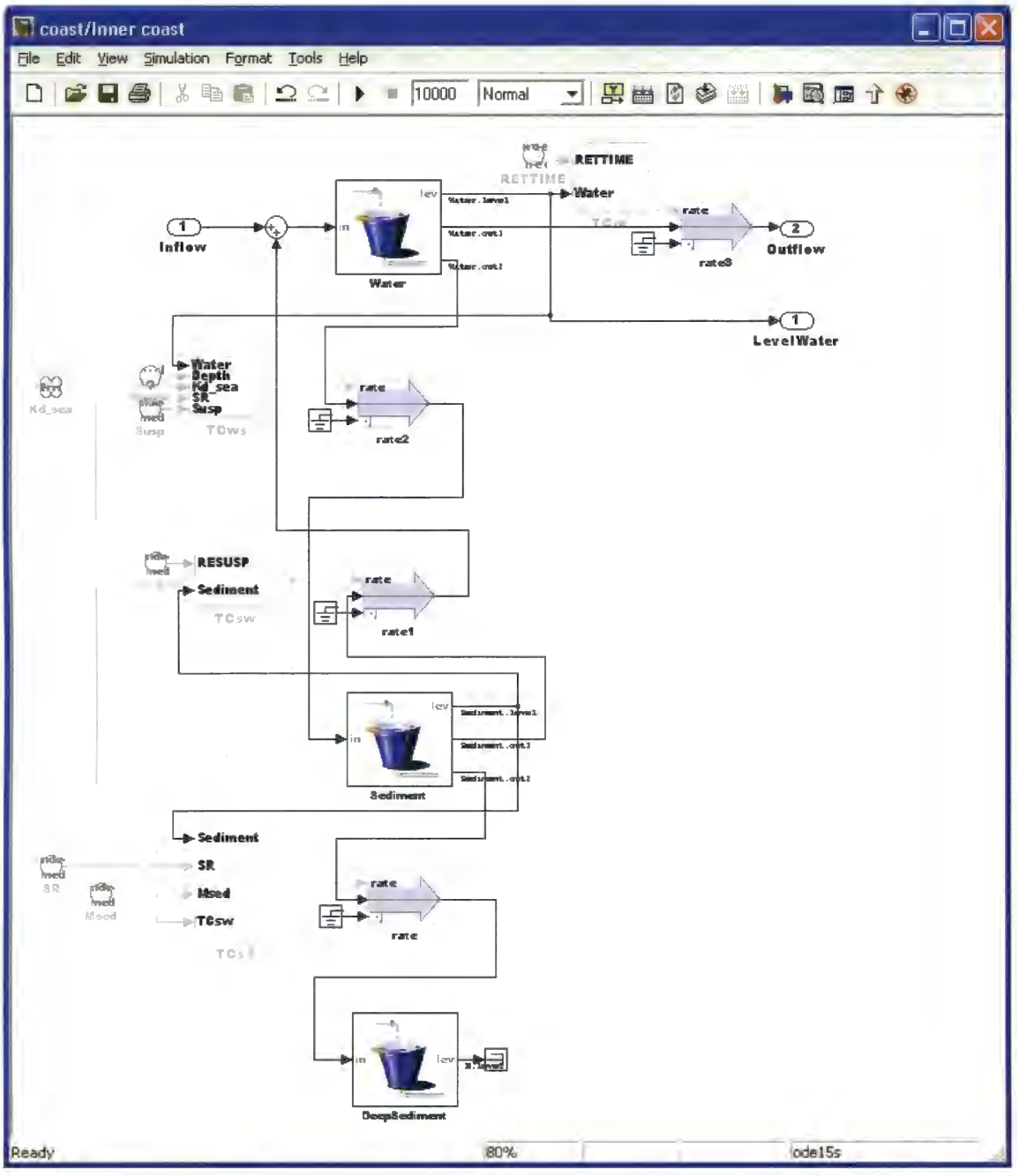

Figure 5.3. *Step 5 of the implementation of the test case model (the Inner coast subsystem).*

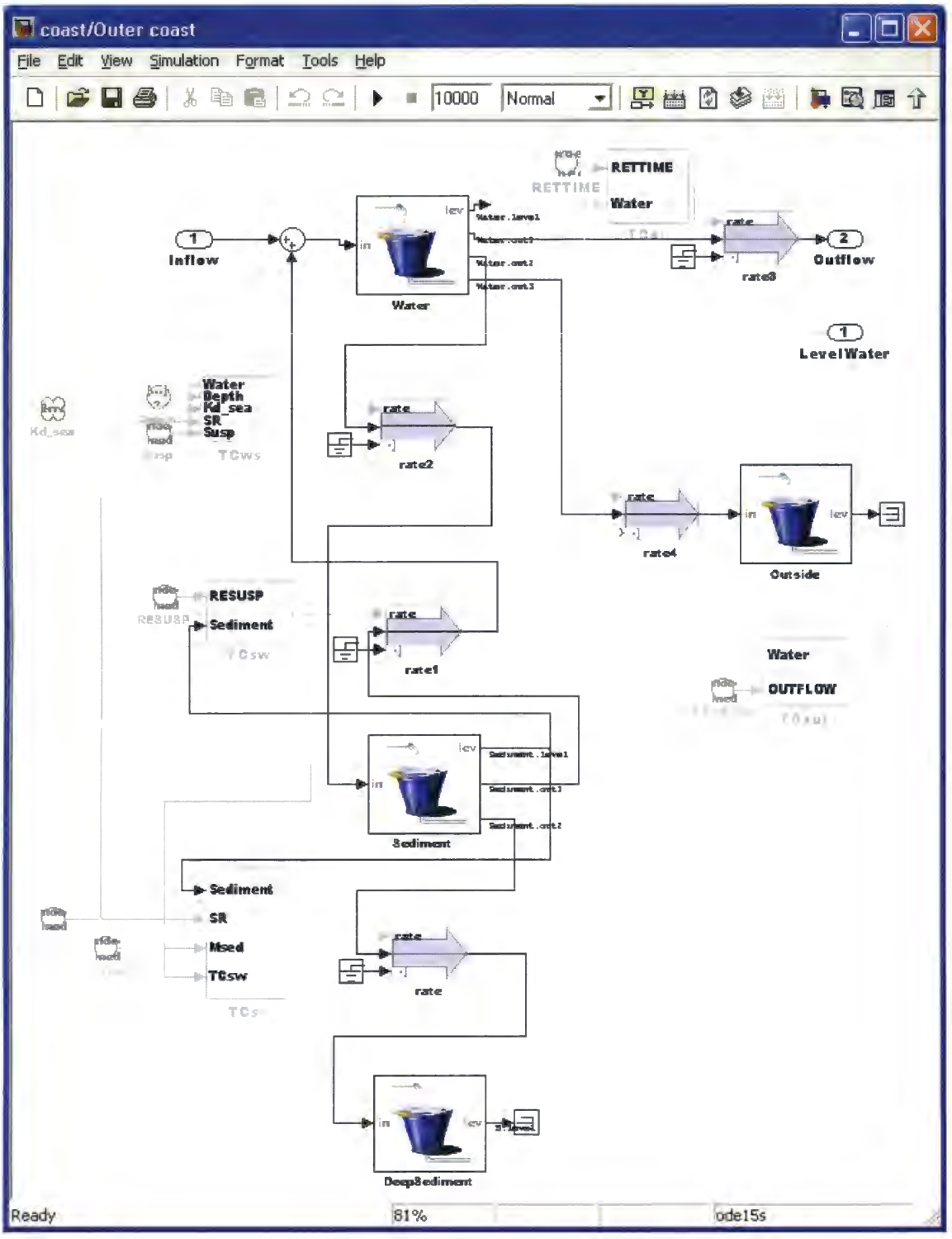

Figure 5.4. *Step 6 of the implementation of the test case model (the Outer coast subsystem).*

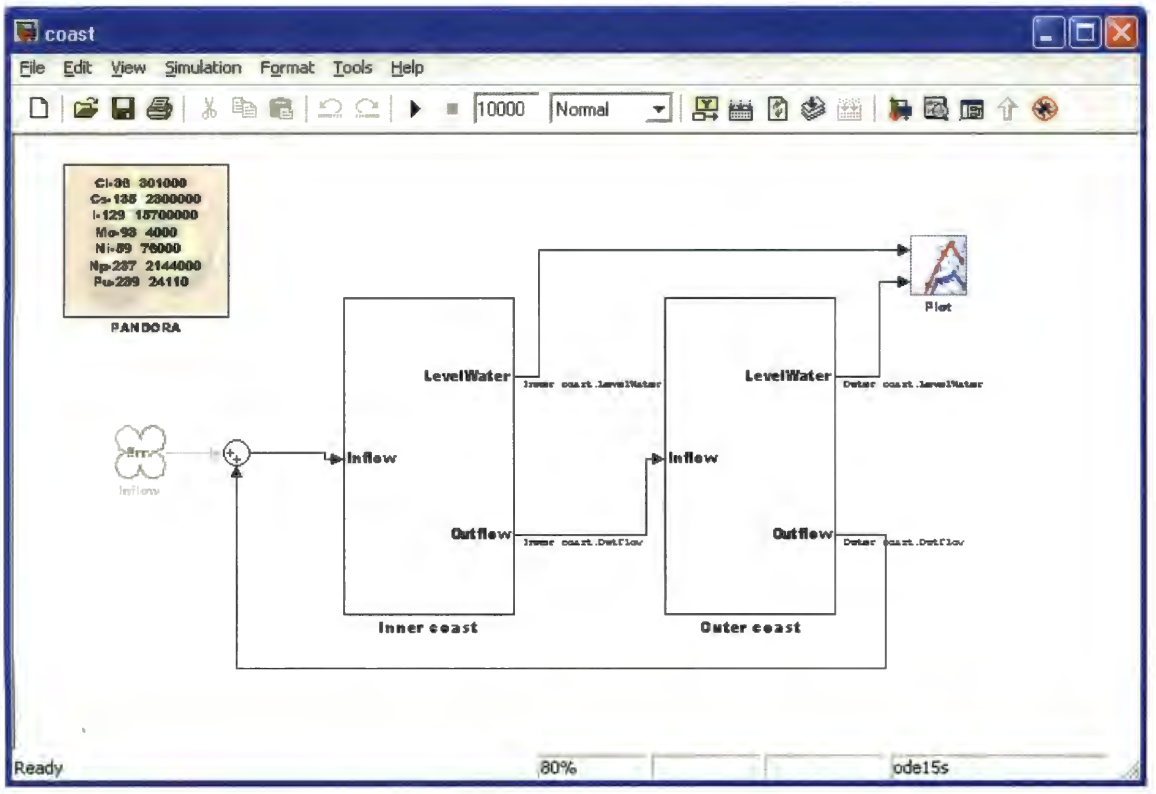

Figure 5.5. *Step 7 of the implementation of the test case model (connection of the subsystems Inner coast and Outer coast).*

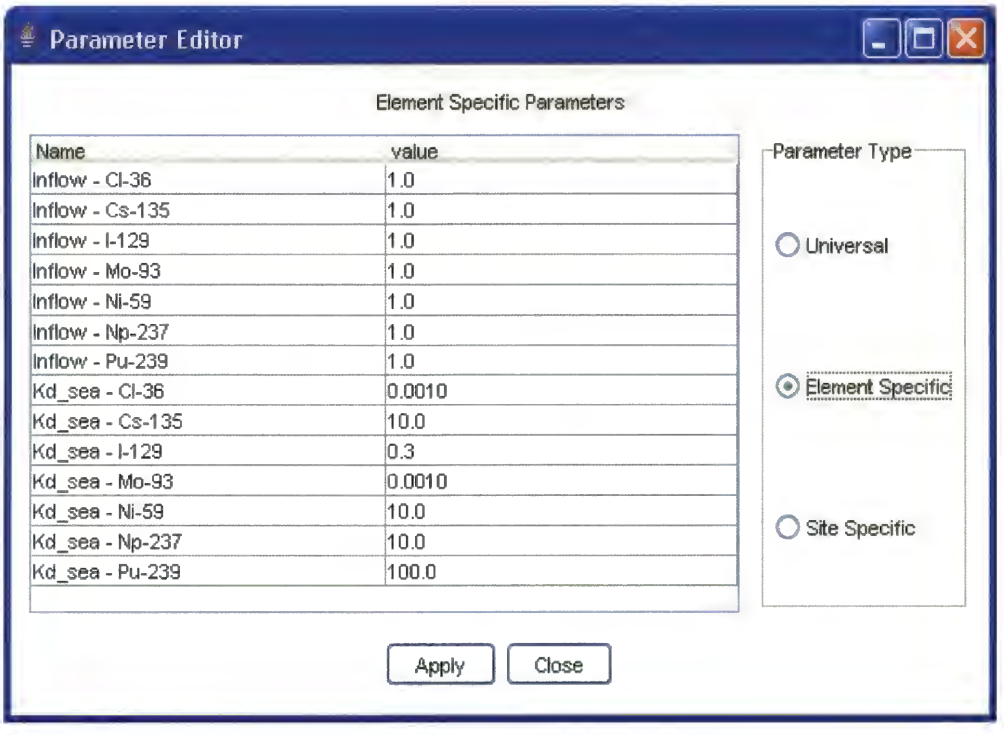

Figure 5.6. *Step 9, phase 1 of the implementation of the test case model (input of element-specific parameters in the Parameter Editor).*

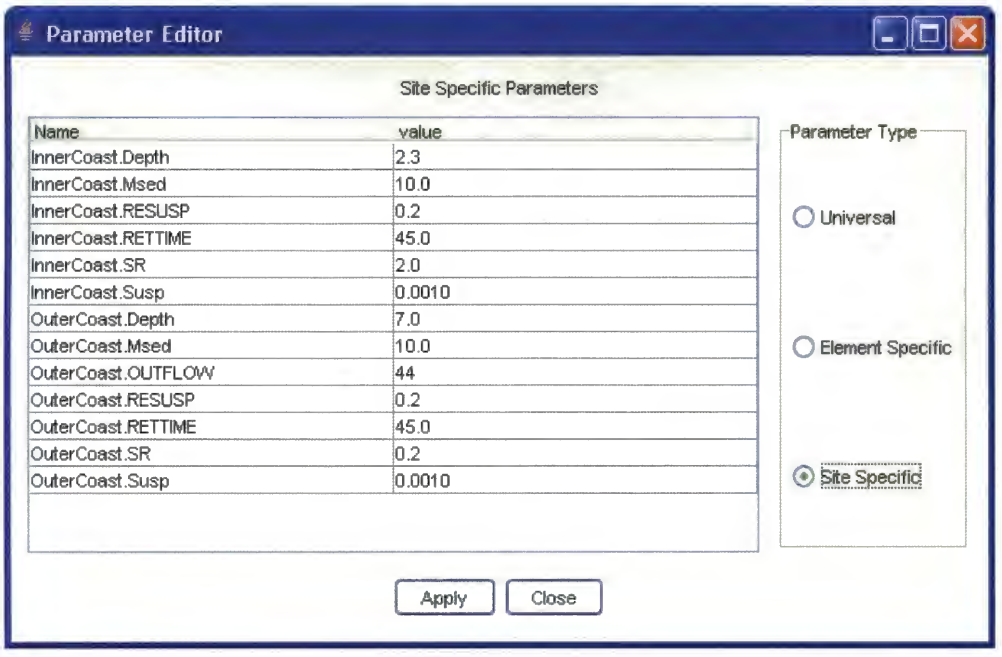

Figure 5.7. *Step 9, phase 2 of the implementation of the test case model (input of site-specific parameters in the Parameter Editor).*

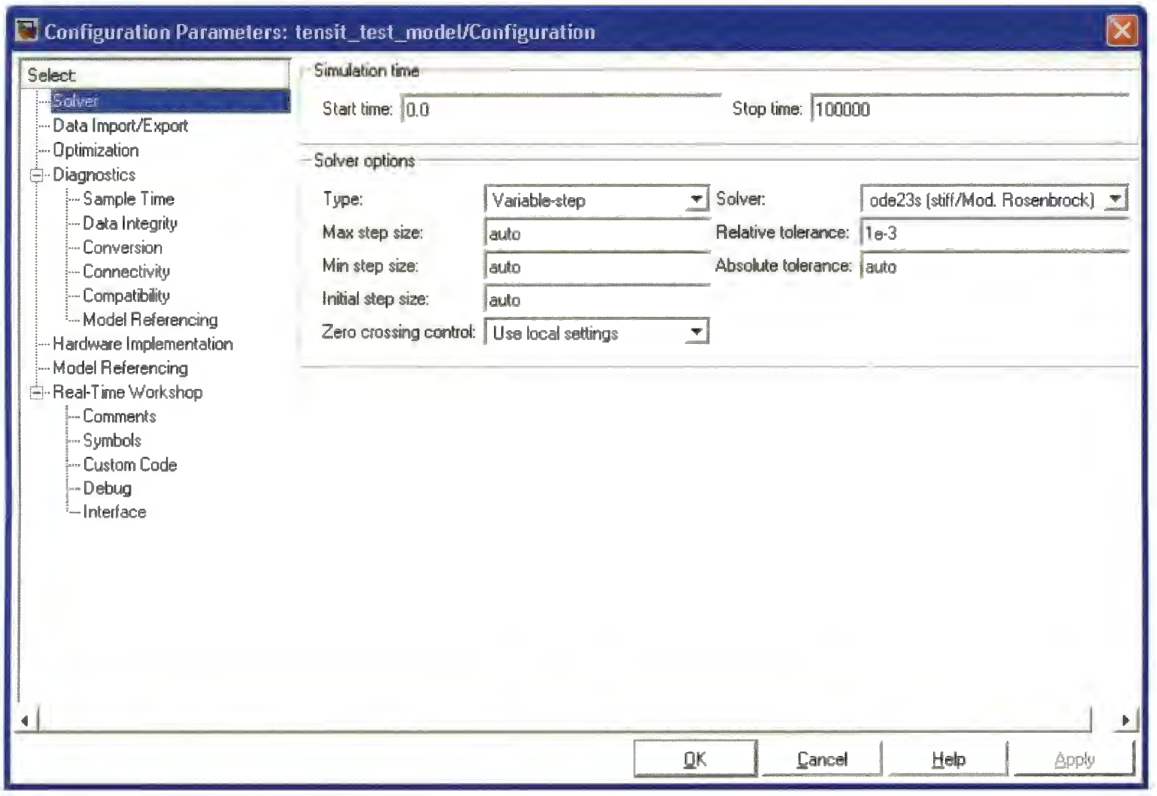

Figure 5.8. *Step 10 of the implementation of the test case model (simulation settings).*

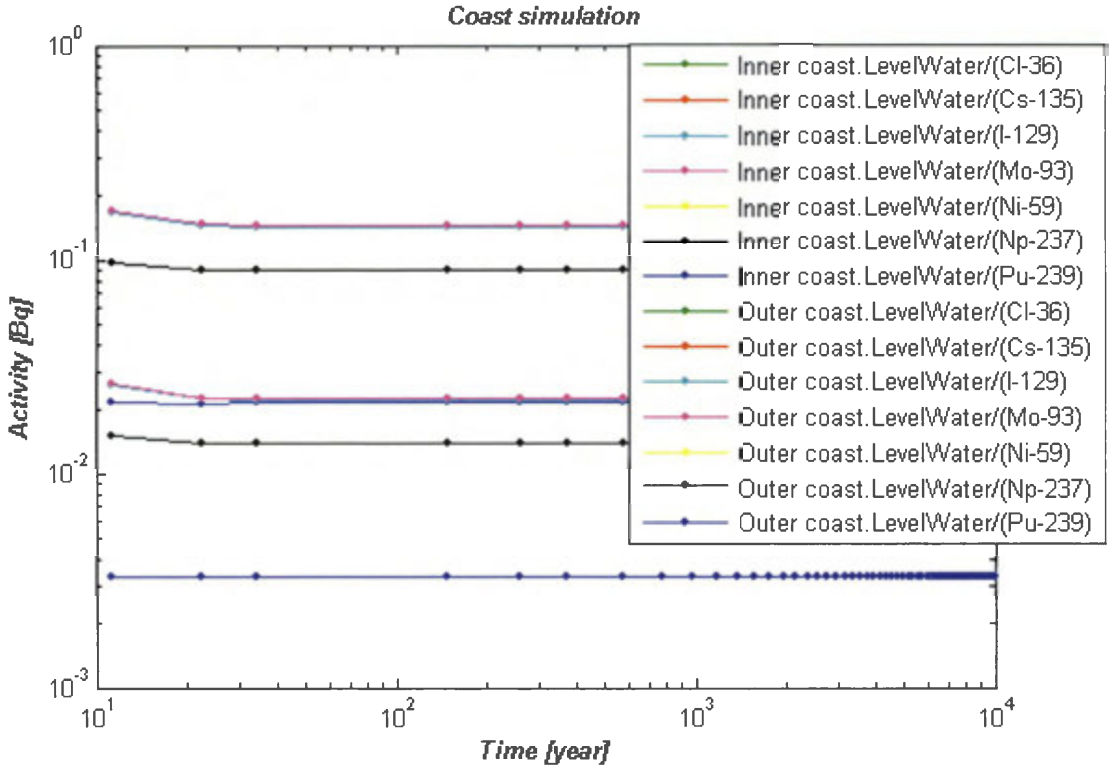

Figure 5.9. *Plot of result from the test case model.*

6 BENCHMARKING, TESTS AND COMPARISONS

Pandora as well as its predecessor Tensit (Jones et al. 2004) has been benchmarked, tested and compared with other similar tools. Ecolego (Avila et al. 2000), another tool based on the Matlab/Simulink software and utilising similar model approach as Pandora, has undergone several comparisons with other tools (Maul et al. 2003). We believe that the successful results from these comparisons are implying also confidence to Pandora.

The predecessor of Pandora, Tensit, was compared with several analytical results as well as numerical results from other simulation tools (Robinson et al. 2003); the comparison is described in Jones et al. (2004).

For testing Pandora version 1, one of the models used in the Tensit tests (SN2, see the references above) was implemented and run as described in section 6.1.

6.1 Implementation of reference model SN2 in Pandora

This model consists of three compartments with a transport of nuclides according to figure 6.1. The calculation takes into account the decay of two nuclides: Nuclide 1 decays at a rate of $1x10^{-4}$ y^{-1} and Nuclide 2 at a rate of $1x10^{-2}$ y^{-1}. The source to A is for Nuclide 1 only and equals zero except for two time intervals: from 0 to 10 years (1 mol/year) and from 30 to 50 years (2 mol/year). The initial transfer rates are given in Table 6.1. After 40 years all transfer rates decrease by a factor of 100.

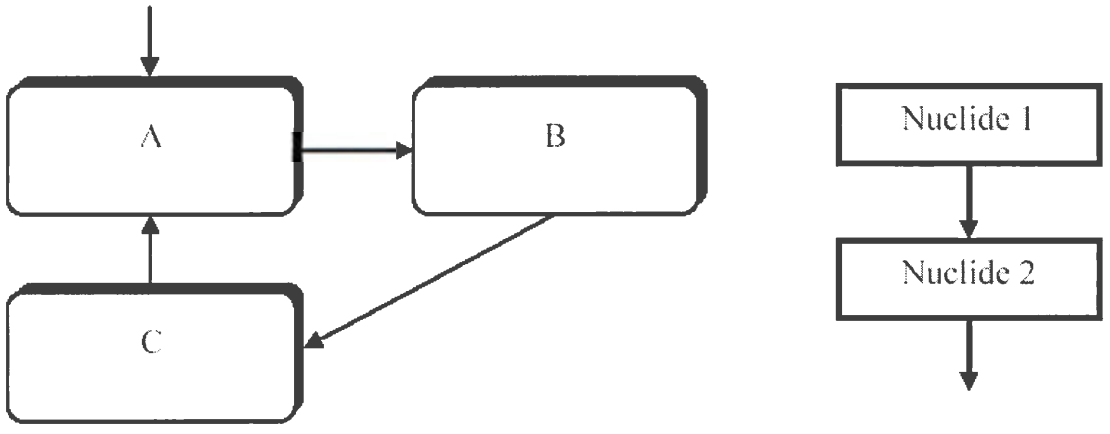

Figure 6.1. *Conceptual representation of the SN2 reference model (Jones et al. 2004).*

Table 6.1. *Initial transfer rates for the SN2 reference model. After 40 years all transfer rates decrease by a factor of 100.*

From	To	Nuclide 1	Nuclide 2
A	B	0.01	0.001
B	C	0.001	0.1
C	A	0.1	0.1

The Pandora implementation (figure 6.2) utilises, in addition to the Pandora blocks, Pulse blocks and Embedded Matlab function blocks from the Simulink library (for further details see the Matlab documentation). The configuration parameters are shown in figure 6.3.

The results of the Pandora implementation are compared to the AMBER calculations (Robinson et al. 2003) after simulation times of 10 and 100 years, as listed in Table 6-2. The results show very good agreement.

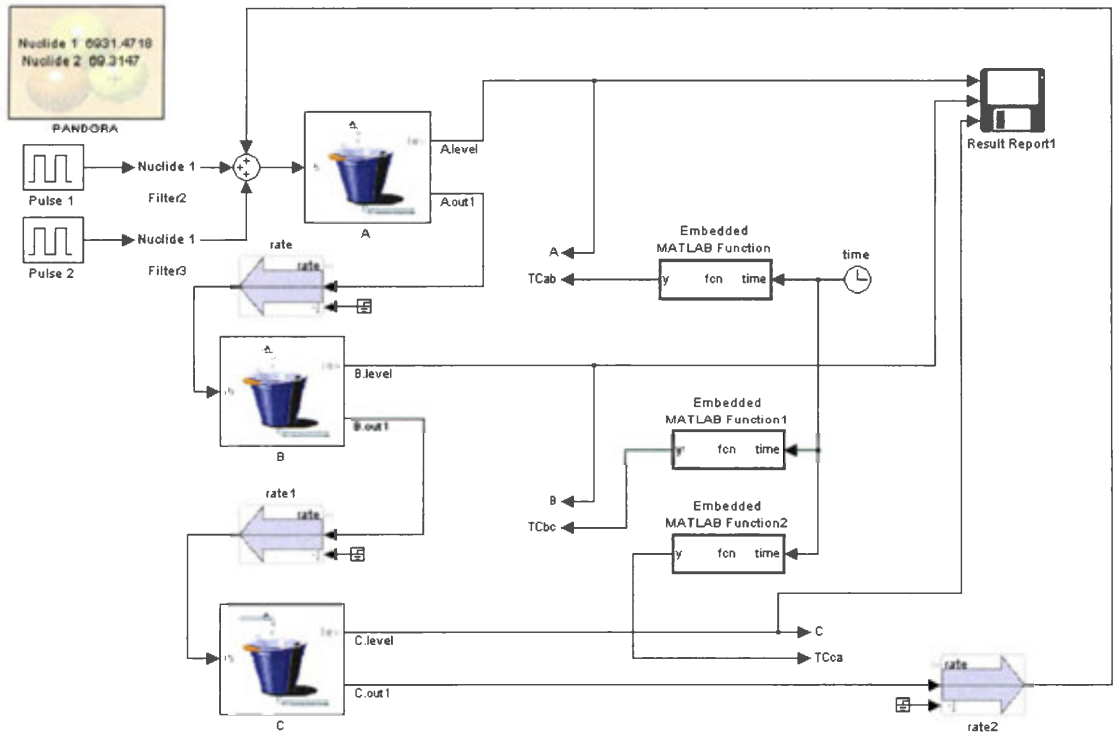

Figure 6.2. *The SN2 reference model implemented in Pandora.*

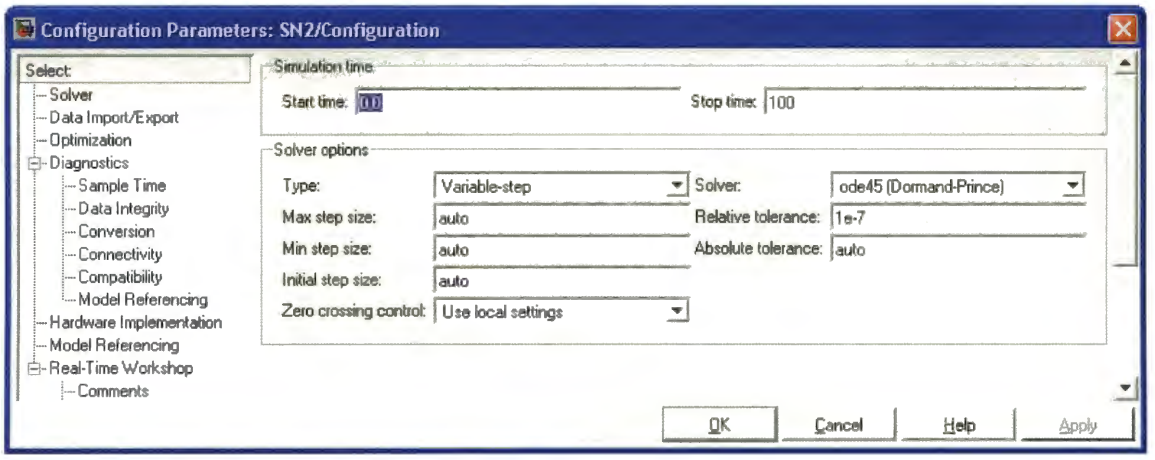

Figure 6.3. *Configuration parameters used in the Pandora test run.*

Table 6.2. *Results of the Pandora implementation and run of the SN2 reference model compared with the results with AMBER (Robinson et al. 2003).*

Compartment	Nuclide	Time [Years]	Results from AMBER	Results from Pandora
A	Nuclide 1	10	9.51191	9.511911532
A	Nuclide 2	10	0.00466821	0.004668213
B	Nuclide 1	10	0.481807	0.481807088
B	Nuclide 2	10	0.000137849	0.000137849
C	Nuclide 1	10	0.00128305	0.001283046
C	Nuclide 2	10	2.97307E–5	2.97308E-05
A	Nuclide 1	100	45.5501	45.55008314
A	Nuclide 2	100	0.220230	0.220230038
B	Nuclide 1	100	4.09113	4.091136749
B	Nuclide 2	100	0.0188336	0.018833612
C	Nuclide 1	100	0.0249555	0.024955533
C	Nuclide 2	100	0.00142203	0.00142203

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APPENDIX A: INSTALLATION OF PANDORA

A.1 Software requirements

Pandora was developed on Matlab7.0.1©, Simulink 6.1©, Windows NT/XP© and Microsoft Excel 97©.

For correct operation of Pandora it is advisable to use these software releases or later ones.

A.2 Installation of Pandora version 1

The Pandora version 1 is delivered in a compressed file *Pandora.zip*. To install the package

1. Unpack the file *Pandora.zip*. When the file is unpacked a directory called *Pandora* is created.
2. Add the path (with subfolders) to this directory e.g. *C:\Pandora* to the Matlab path. This is done from the *File > Set Path* menu in Matlab.
3. You should now be able to see the Pandora library in the Simulink library browser as in Figure A.1.

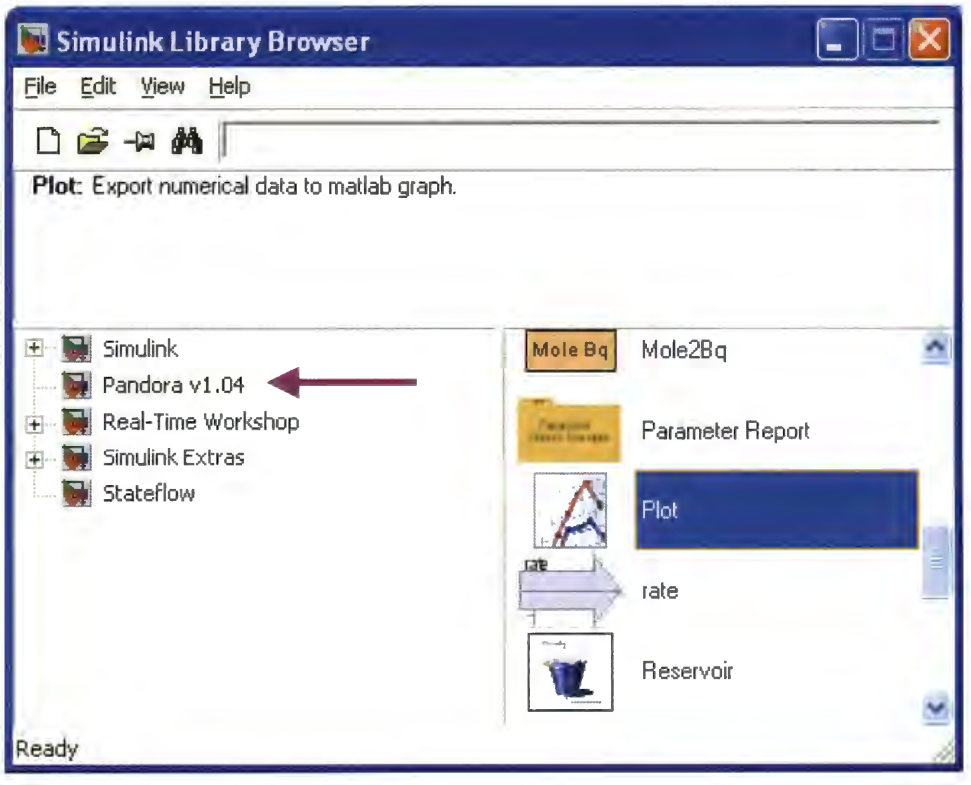

Figure A.1. *Pandora in the Simulink library browser.*